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NBS TECHNICAL NOTE 1214

U.S. DEPARTMENT OF COMMERCE/National Bureau of Standards

NBS * LATTICE

A Program to Analyze Lattice Relationships

Vicky L. Himes and Alan D. Mighell

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No. 1214
1985
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NBS Technical Note 1214

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A Program to Analyze Lattice Relationships

Version of Summer, 1985

Vicky L. Himes and Alan D. Mighell

NBS Crystal Data Center
Reactor Radiation Division
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NBS*LATTICE

A Program to Analyze Lattice Relationships
Version of Summer, 1985

Vicky L. Himes and Alan D. Mighell

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A FORTRAN program to analyze lattice relationships has been written and is available for distribution by the NBS Crystal Data Center. The present version of *NBS*LATTICE* performs several functions including: 1) the characterization and identification of unknown materials using lattice-formula matching techniques; 2) the calculation of the reduced cell of the lattice, and the calculation and reduction of specified derivative supercells and/or subcells (i.e., this program function calculates the standard cells which are useful in the determination of metric lattice symmetry, in finding a matrix relating two unit cells, etc.); 3) unit cell transformations; and 4) matrix inversions. It is planned to incorporate additional functions in forthcoming versions of this program. Among others, these functions will include a matrix method to determine metric lattice symmetry and a technique to find a transformation matrix relating any two unit cells.

Key words: computer program; lattice; identification; reduction; supercell; subcell; symmetry; transformation; data base.

I. Introduction

The NBS Crystal Data Center has been compiling crystallographic data for approximately 20 years. Over the years, the Data Center has developed a number of evaluation procedures that can be used to analyze lattice relationships. These techniques would also be useful to the general scientific community. Consequently, a computer program based on these procedures has been written and is being distributed by the Data Center. This work is being supported by the Office of Standard Reference Data at NBS and the JCPDS-International Centre for Diffraction Data.

The *NBS*LATTICE* program is written in standard FORTRAN and is designed to be used in any analytical laboratory. The software is multifunctional and can be used to analyze various types of lattice relationships. For example, when the program is used with the *NBS Crystal Data File* (1982), one can characterize and identify unknown materials based on lattice-formula matching techniques. In addition, reduced cells and reduced derivative supercells and/or subcells can be calculated by the program. Thus, this program function calculates the standard cells which are useful in determining metric lattice symmetry, in finding the relationship between two unit cells and in the identification of unknown materials. In addition to the more complex functions, the program performs simpler calculations which are useful in routine crystallography. With the program, for example, one can find the inverse of a three by three matrix and transform a unit cell by a specified matrix. It is planned to incorporate additional program functions in forthcoming versions of *NBS*LATTICE*. Among others, these include a matrix technique for metric symmetry determination and a method to find a transformation matrix relating any two unit cells.

The examples of lattice relationships discussed in this manual are actual problems. Many have been published previously (Himes, 1983 and references cited therein).

II. Identification by lattice matching

A. Introduction

The lattice-matching program function is designed to be used in conjunction with the *NBS Crystal Data File* (1982) for the characterization and identification of crystalline materials. The NBS Crystal Data Center maintains a data base that contains evaluated crystallographic and chemical data on approximately 60,000 materials. The data fall into the following categories: organics, organometallics, metals, intermetallics, inorganics and minerals. There are two fundamental ways that large crystallographic data bases can be used. As a source of critically evaluated data, the data base can be used as a basis for scientific research, or as an aid to scientific research (e.g., to identify unknown compounds, to locate certain molecules, to obtain bibliographic data, etc.). The type of data that can be obtained through search and retrieval programs include chemical name and formula, cell parameters and cell volume, crystal system, space group symbol and number, density, bibliographic data, plus additional data. Since the data base is formatted, many of these data items may be searched readily using systems software available at a particular institution. However, general systems software will not be adequate for certain types of information search and retrieval operations. One such example is the identification of unknown compounds by matching lattices (as defined by unit cell parameters) and, if available, some chemical data. Although simple in principle, lattice-formula matching is a complex operation that requires specialized scientific background in order to design a practical computer search algorithm. The following section summarizes the lattice-matching technique developed at NBS. It is planned to incorporate the formula-matching operation in a subsequent version of this program.

Three relatively recent developments have given the lattice-formula method for compound identification great potential as a routine analytical tool. First, automated methods to determine a unit cell (and crystal structure) are in widespread use. For the same reason, the data base of known crystalline compounds is large and is rapidly growing. Second, new mathematical theories have practical applications in lattice-matching procedures. These procedures permit fast and effective identification in spite of certain experimental errors made in unit cell determinations. Third, advancements in computer technology have greatly increased the efficiency of search strategies through direct access of computer file records and increased mass storage capability.

B. Background and theory

The identification of materials by powder diffraction is a well-established analytical technique. With the powder method, identification is based on matching the many diffraction positions and intensities with those of known materials. In contrast, the method described in this Section identifies materials based on their crystalline lattices as defined by the unit cell parameters. Matching unit cell parameters may be thought of as matching all possible positions of the diffraction lines (d-spacings) in a powder pattern. Practically, however, there are many advantages to the lattice-matching approach, mainly due to the very compact nature of the unit cell as compared to a powder pattern. For example, it is far easier to treat the experimental errors when matching unit cell parameters than it is to evaluate the errors in all the observed (and unobserved) diffraction positions in a powder pattern. In addition, the computer search times and mass storage requirements are significantly decreased since there are fewer search parameters for the lattice-matching method. Finally, with a given unit cell, mathematical procedures allow one to calculate derivative unit cells which could result from certain errors made by the experimentalists. Since the lattice-matching method is efficient, one is able to routinely search the data base of known materials for the experimentally determined unit cell as well as for its calculated derivative cells.

There are many unit cells that can be chosen to define a crystalline lattice. When identifying a material using the powder method, unique sets of data are matched since any unit cell defining the lattice gives the same calculated d-spacings. With the lattice-matching method, this uniqueness is guaranteed by always comparing reduced cells. The reduced cell is a unique, primitive cell based on the three shortest lattice translations and satisfying a specified set of mathematical conditions. (Section III describes the reduction and derivative lattice theory and applications.) For identification, each unknown cell and, if calculated, each of its associated derivative cells is transformed to a reduced cell. These reduced cells are then checked against a reduced cell data base of known materials.

The NBS Crystal Data Center has prepared a data base that can be used for compound identification and characterization. The *NBS Crystal Data File* is described more fully in Appendix I. In this File, all known cells have been transformed to a reduced cell and the File has been sorted first on increasing magnitudes of the unit cell parameters. With this classification scheme, metrically similar lattices are located near each other in the File, making it possible to design efficient lattice-search algorithms.

A summary of the lattice-formula matching procedure is presented in figure 1. From the unknown crystal, a unit cell is determined and reduced. The reduced cell is then checked against a file of known materials. If desired, one calculates derivative lattices which are also reduced and checked against the File of knowns. Finally, the identification is verified using known chemical data. This procedure can be carried out either by hand using a printed listing of knowns, or by computer program. Practical examples of this identification procedure are illustrated in figures 2 and 3.

In figure 2, only one single crystal of the sample was available. Thus, a chemical analysis was not possible. The initial cell was determined on an automated diffractometer. This C-centered cell was transformed to a primitive cell and reduced. The reduced cell was then checked against the *NBS Crystal Data File*. The sample was found to be sodium sesquicarbonate dihydrate by a direct match of the reduced cell parameters. A full structure determination by neutron diffraction confirmed the identification (Choi & Mighell, 1982).

The example given in figure 3 shows how an identification can be made by using a derivative lattice procedure. In diffraction work, one may determine a supercell or subcell rather than the correct cell of the lattice. For example, when using powder methods, a supercell in direct space may be determined if one does not find the smallest cell consistent with the set of d-spacings. In single-crystal work, a subcell in direct space is determined if reciprocal lattice nodes are missed on a diffraction photograph or a diffractometer. In either case, it is possible to systematically calculate derivative cells and identify the material. Here, the unknown cell was correct and the known cell was a supercell. The initial cell and space group were determined on a single-crystal diffractometer and a full set of diffraction data was collected. The empirical formula was known. When checked against the File of known compounds, there were no matches. Next, the seven supercells of twice the volume were calculated; only three were unique because the initial cell is metrically rhombohedral. One of the three calculated supercells matched a cell in the *NBS Crystal Data File*. The known cell, which was a supercell of the correct cell, had been determined from powder data only. Nevertheless, it was possible to verify the correct composition and to find appropriate literature references.

Figure 1. *Identification by lattice-formula matching*

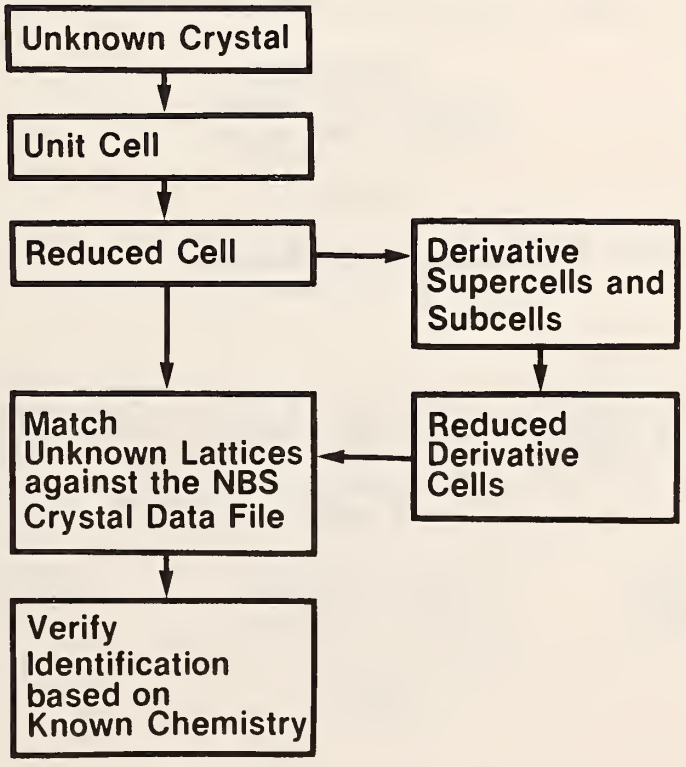
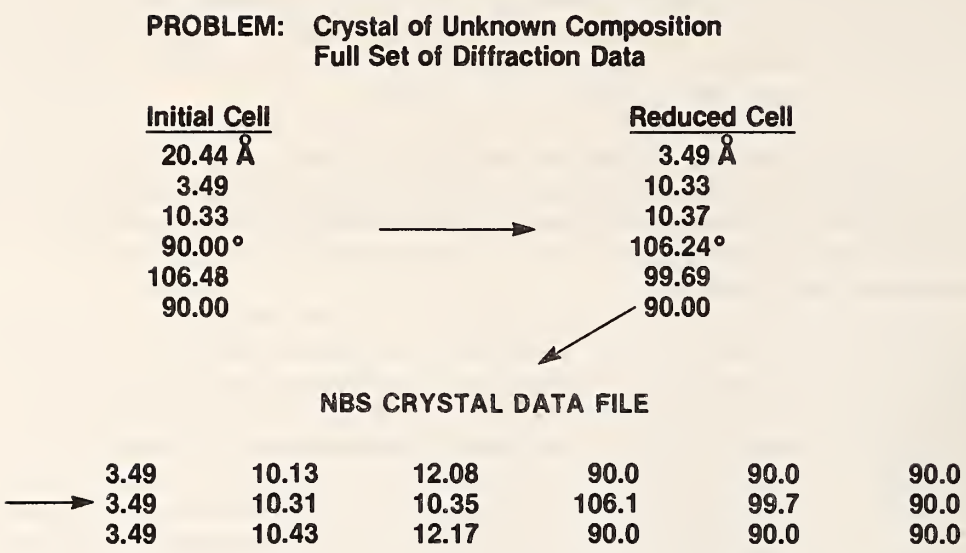
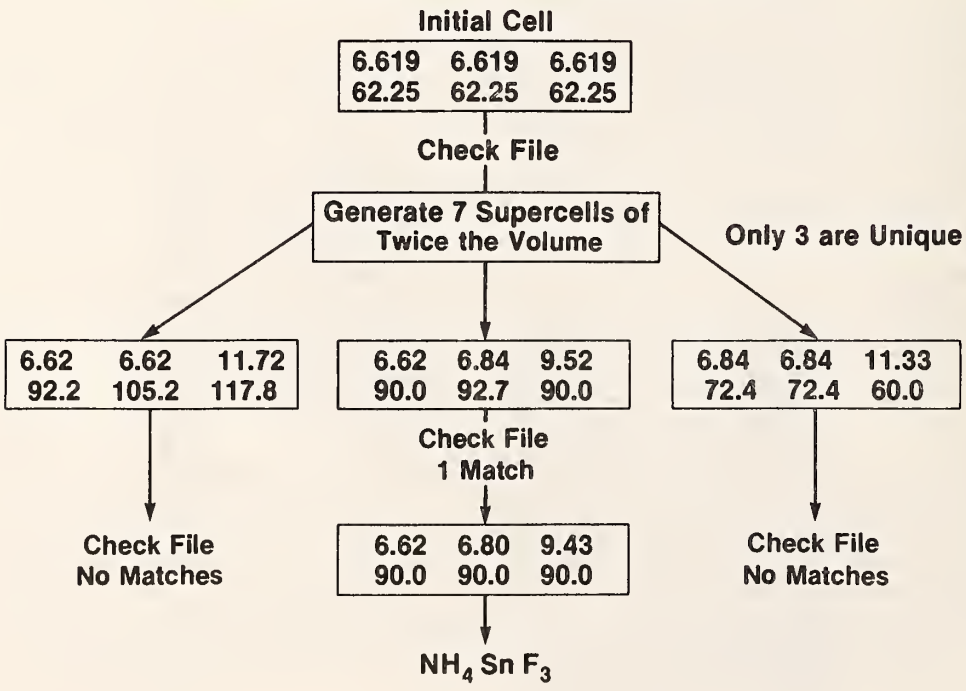


Figure 2. *Identification: direct cell match*



* The cell parameters shown represent three adjacent file entries, not three separate matches.

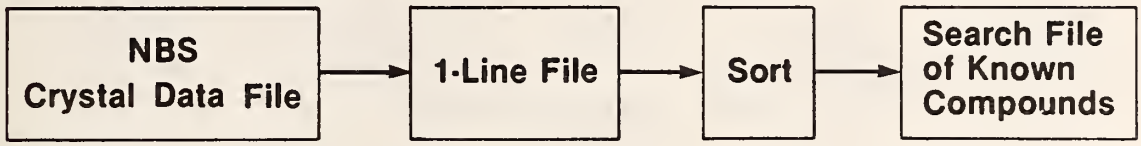
Figure 3. *Identification: match of a derivative cell*



C. Algorithm

The theoretical basis for identification by lattice-formula matching was briefly discussed in the previous sections. Here, emphasis is placed on the computer strategy used to match the unknown lattice(s) against the *NBS Crystal Data File.*

1. Preparation of a search file of known compounds



Before using the NBS lattice-matching program function, a compact search file of known compounds must be prepared. This is done to save computer mass storage, to increase the efficiency of a search, and to simplify the program's input and output operations. Selected data from the *NBS Crystal Data File* are used to create a search file in which each line of 132 characters corresponds to the data for one crystalline compound. For a given computer, the 1-line search file is prepared only once.

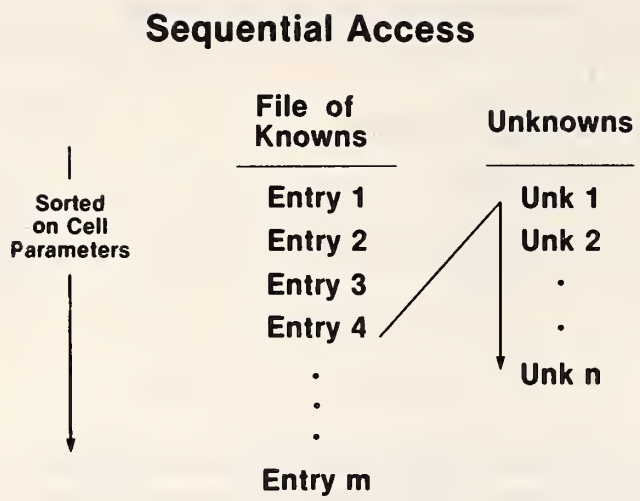
Data Items in the Search File of Known Lattices

Reduced Cells

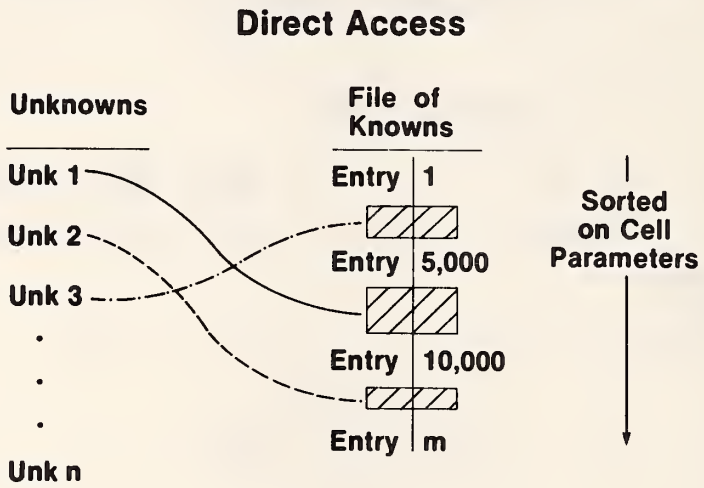
Increasing Cell Parameters

a	b	c	α	β	γ	V	SG #	Ref.	Formula
a_2	b_2	c_2	α_2	β_2	γ_2	V	SG #	Ref.	Formula
a_n	b_n	c_n	α_n	β_n	γ_n	V	SG #	Ref.	Formula

In the 1-line search file, each known lattice, regardless of its original centering, is represented by its primitive, reduced cell. The entries are ordered by increasing magnitudes of the reduced cell parameters. The space group, literature reference, chemical formula and other information are included in order to facilitate identification. A description of the data items and format specifications for the 1-line search file are given in Appendix II.

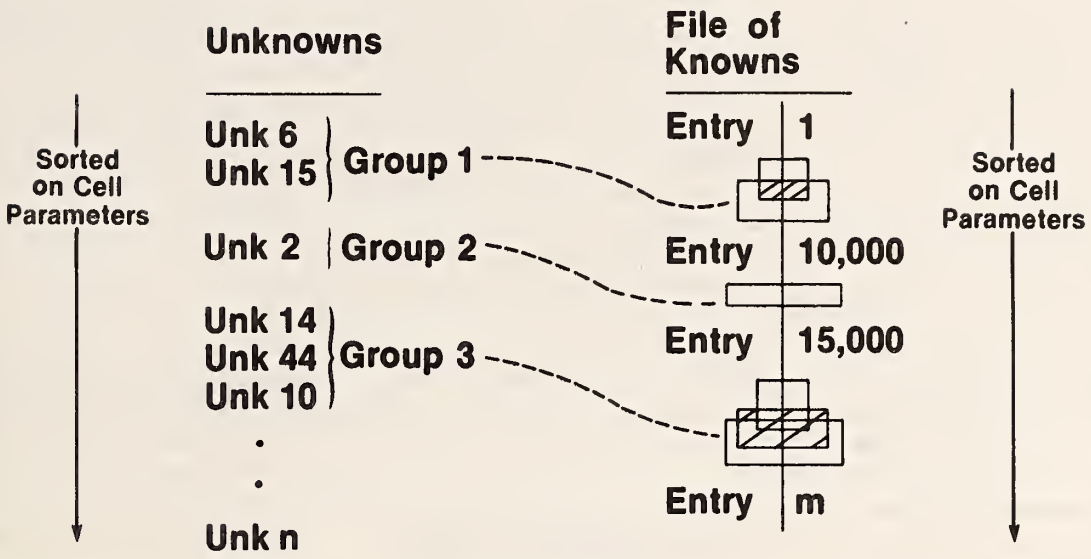


When matching an unknown against a file of known compounds, two different strategies can be used to access the computer files: sequential and direct access. In the sequential access approach, one reads from the beginning to the end of the file of knowns in a 'forward' manner only. After each read, a given file entry is matched against all the unknowns.



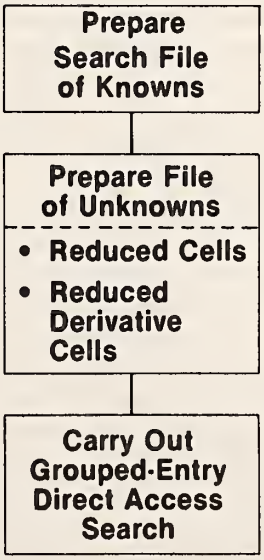
Unlike sequential access files, direct access enables one to go directly to a specified point in the file. One can access the file in any order, 'forwards' or 'backwards'. The direct access of file records is efficient as it can significantly decrease the number of file reads. The 1-line search file used for identification is a direct access computer file. In this direct access code, a knowledge of the data in the file of knowns is used to set up a system of pointers which allows the program to start searching in about the right region of the data file. A sequential search is used only for the regions of the file in which a match is possible. In the diagram, the search regions are designated by boxes.

Grouped-Entry Direct Access



A 'grouped-entry' direct access search strategy is actually used in the *NBS*LATTICE* program. To carry out a grouped-entry direct access search, the unknowns are first sorted on increasing values of the reduced cell parameters. Duplicate lattices (i.e., those with exactly the same a,b,c,alpha,beta,gamma) are then deleted for the sole purpose of eliminating repetitive output. Next, unknown cells with similar values of a (Å) are searched as a group against the appropriate region of the data file. In the diagram, the regions that overlap are searched only once. This approach is very efficient when one searches a number of unknowns against the 1-line search file.

Grouped-Entry Direct Access Search



The above diagram summarizes the lattice-matching procedure developed at NBS. First, the 1-line search file of knowns is prepared from the *NBS Crystal Data File*. For a given computer, this direct access file of knowns is prepared only once. Second, the file of unknowns is prepared. Each input cell may be a primitive or centered cell of the lattice. Derivative supercells and subcells may be calculated from the input cell. All cells in the file of unknowns are reduced and sorted on increasing values of the reduced cell parameters (see sec. III for details on the reduction and derivative lattice calculations). Third, the grouped-entry direct access search is carried out. Each unknown cell as well as derivative supercells and subcells may be matched against the file of knowns in a single run.

3. Lattice-matching strategy

There are two basic strategies that can be used to determine whether two unit cells define the same lattice: the cell and the matrix approaches. The present version of the *NBS*LATTICE* program uses the first strategy. The experimentally determined unit cells for both the known and unknown compounds are converted to standard, reduced cells. The reduced cell parameters are then compared; if the reduced cells are the same, then the original cells define the same lattice. Reduction is a mathematical procedure that leads to a unique cell in all cases, provided there is no experimental error in the unit cell parameters. However, as explained in section III, occasionally, the computer program may yield a geometrically reduced cell that requires further reduction with respect to the cell angles because of the interactions of the experimental errors with the normalization procedure and the process of satisfying the special conditions for reduction. Thus, in practice, two experimentally determined cells defining the same lattice will always give the same a,b,c (within experimental error) for the reduced cell, but in certain cases, the reduced cell angles may differ. For this reason, the program matches only the cell edges and cell volume of each unknown reduced cell against the known cells in the *NBS Crystal Data File*. It is possible that every match obtained in this way does not define the same lattice. In the next version of the program, a mathematical procedure (Santoro, Mighell & Rodgers, 1980) will be used to distinguish between lattices that have only a,b,c,V in common and lattices that are identical. For those cases in which more than one match of a,b,c,V occurs, knowledge of the empirical formula or some other chemical information is almost always sufficient to eliminate unwanted matches. This chemical screening will be automated in a later version of the computer program, completing the identification procedure by lattice-formula matching.

D. NBS Crystal Data File: selectivity and nature of the data

The *NBS Crystal Data File* contains evaluated crystallographic and chemical data on approximately 60,000 materials. For convenience, these data have been divided among two separate 1-line search files, one composed of 'organic' data and the other containing 'inorganic' data. Each search file contains approximately 30,000 entries. Certain differences have been noted in the space group frequency distributions of the organic and inorganic data (Mighell, Himes & Rodgers, 1983; Mighell & Rodgers, 1980). The compounds in the organic search file usually crystallize in the lower symmetry crystal systems; while the space groups for materials in the inorganic search file are skewed towards the higher symmetry crystal systems. This has practical implications in the identification of compounds. For organic compounds, the cell alone (a,b,c,V) is usually sufficient to fully characterize the material. However, because the inorganic search file generally contains more compounds from the higher symmetry crystal systems and a greater percentage of isostructural data, some chemical information is often needed to fully characterize these materials.

Experience has shown that the unit cell is highly characteristic of a compound and, like a powder pattern, may be used for identification. On the average, only $\sim$500 entries in either the organic or inorganic search file will separate two entries when the a-values of the reduced cells differ by $\sim$0.20 to $\sim$0.25 Å. In the middle region of each search file, $\sim$500 file entries will separate two reduced cells whose a-values differ by $\sim$0.11 Å. Thus, the lattice-matching procedure is relatively selective based on the a-cell parameter alone. When values of b, c and V for the reduced cell are considered, the selectivity is dramatically increased. (The selectivity will be further enhanced in the next version of the program by the addition of a mathematical technique to distinguish between lattices that have only a,b,c and V in common and lattices that are identical.)

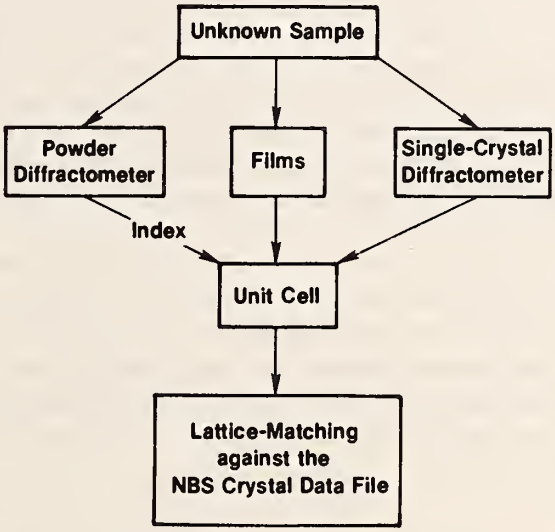
As part of a practical test of the lattice-matching method, the entire 1-line organic search file ($\sim$30,000 compounds) was considered as a file of unknowns to be matched against itself. When tolerances of $\pm$0.1 Å for a,b,c and $\pm$10 percent for V were used, most 'unknowns' gave only one or two matches. In the entire analysis, a maximum of 17 matches of a,b,c,V were found for a single 'unknown'. These contained data for the same or isostructural compounds. As expected, a similar analysis of the inorganic search file yielded more matches on the average. These two analyses demonstrated the efficiency of the computer program as well as the selectivity of the lattice-matching method.

E. Concluding remarks

The identification of an unknown compound can be highly automated including the determination of the unit cell. Both the unit cell determination and the identification process can be carried out in one instrument.

The lattice-matching method of identification is ideal for automated analyses since it is subject to precise mathematical procedures. The method is efficient, highly selective, and various types of inter- and intra-lattice relationships can be established. In practice, the technique is reliable as the *NBS Crystal Data File* contains evaluated data on well-characterized materials. Usually, the cells have been refined by least-squares techniques and the chemistry is precisely known. For most crystals, the lattice is unique. This means that the cell or the cell plus some chemical data is sufficient for identification. Experience with practical problems has shown that identification by matching reduced cells is very straightforward and reliable when the correct cell of the lattice has been determined. However, a material can often be identified even if an error has been made in which a derivative cell of the unknown has been found. For example, if the cell centering is missed when indexing a powder pattern or, when using single-crystal methods, if rows of spots are missed on the diffraction photographs, this would result in the determination of a derivative cell of the correct lattice. To make an identification, one systematically calculates the derivative supercells and subcells and looks for matches in the *NBS Crystal Data File*. When searching for matches, relatively large tolerances are used routinely. In addition, checks for the 55 supercells of 2,3, and 4 times the volume of the unknown reduced cell and the 55 subcells of 1/2,1/3, and 1/4 times the volume are made. The ability to check routinely for matches of 110 extra derivative cells for each unknown is only possible because of the efficiency of the computer program and the selectivity of the method.

Lattice-Matching Method for Identification



As the above diagram illustrates, the lattice-formula method of identification is a general procedure that may be applied to any cell regardless of the technique used for its determination, including x-ray, neutron and electron diffraction. The data may be recorded using a single-crystal or powder diffractometer, or by using film methods. In the past, lattices, as defined by unit cells, have not been used for the identification of materials. Traditionally, the experimentalist would grind the sample or employ a Gandolfi camera to obtain a powder pattern; the compound is then identified based on matching observed d-spacings and intensities. However, there are many advantages to the lattice-matching method of identification as compared to the traditional approach. First, the cell gives more information about the metric lattice than a set of d-spacings. A unit cell may be used to calculate a set of all possible d-spacings, but a set of d-spacings may be consistent with more than one cell. Practically, this situation is made worse since a limited set of d-spacings may be observed with the powder method due to the nature of the compound and to other experimental conditions. Second, from the unknown unit cell, mathematical procedures allow one to calculate derivative cells which can be checked against the file of known lattices. Related materials can be found using this strategy, and identification can be made in spite of certain errors made by the experimentalists. Third, it is far easier to treat experimental errors when matching unit cell parameters than it is to evaluate the errors in all the observed (and unobserved) diffraction positions in a powder pattern. Finally, computer search times and mass storage requirements for

identification based on lattice matching are significantly decreased since there are fewer search parameters. In view of its many theoretical and practical advantages, we feel that the lattice-matching technique will change the way in which powder experimental data will be used to identify materials. A unit cell will be determined along with the powder diffraction pattern. The cell may be obtained from an indexing program using the observed d-spacings, or it may be obtained directly using a single crystal taken from the sample. Once a cell has been determined, the identification may be carried out by lattice matching, followed by comparing the powder intensity data and any available chemical information. The identification based on matching d-spacings and intensities should be reserved for those cases in which a lattice match was not obtained, for mixtures, and for those cases in which a unit cell could not be determined. Thus, the ability to identify crystalline materials will be significantly improved due to the general nature of the lattice-matching approach, and the availability of the *NBS Crystal Data File*, a large file containing known lattices from all areas of the solid state.

F. Operation of the Program

1. General

There are three types of input lines required to execute the lattice-matching (LM) program function. The first input line is a Program Control Line that specifies the type of program function and the number of independent problems to be considered. The second input line is an LM Parameter Line that specifies the tolerances for a match of a,b,c, and V, the files to be searched (organic or inorganic), and whether full or limited output is desired. The third type of input line is an RSS (reduction and derivative supercell and subcell; see sec. III) Control Line that defines the input lattice and specifies the derivative lattices to be calculated. For N problems specified on the Program Control Line, one LM Parameter Line and N RSS Control Lines must follow ($1 \leq N \leq 20$). Within a single computer run, the LM program function may be executed only once. Although at most 20 independent problems may be considered, up to 900 lattices, including the unknown lattice(s) plus calculated derivative lattices, may be matched against data from the *NBS Crystal Data File* in a single run. A description of the file assignments, formats for the input lines, and typical examples for the execution of the LM program function follow.

2. Files and file assignments

Before the LM program function can be executed, the *NBS Crystal Data File* must be used to create the direct access 1-line search files. For a given computer, the search files are prepared only once. The filename NBSI must be associated with the inorganic data, while the filename NBSO must be associated with the organic data. A summary of the assignments made when executing the LM program function is given below.

Unit Number	Associated Filename(s)	Description
7	NBSI, NBSO	Direct access 1-line search file
10	NBS10	Scratch file of reduced cell(s) and reduced derivative cells calculated by the program

3. Description of input lines

a. Program Control Line

The Program Control Line specifies the type of program function and the number of independent problems to be considered. To execute the LM program function, one Program Control Line is required.

Program Control Line
Format(A5,3X,I2)

	Column	Format	Item
1	1–5	A5	Type of program function 'LM ' = Lattice Matching 'RSS ' = Reduction and Derivative Supercell and Subcell 'TRANS' = Cell Transformation 'INV ' = Matrix Inversion
	6–8	3X	Blank
2	9–10	I2	Number of problems

Notes:

1 The LM program function is specified by 'LM ' in columns 1–5.

2 The number of independent problems specified for the execution of the LM program function may range between 1 and 20. However, up to 900 lattices, including the unknown lattice(s) plus calculated derivative lattices, can be searched against the file(s) of known compounds in a single run. If more than 900 lattices are generated as a result of the data on the RSS Control Lines, only the first 900 lattices will be used in the lattice-matching procedure.

b. LM Parameter Line

The LM Parameter Line specifies the tolerances for a match of a,b,c, and V, the file(s) to be searched, and whether full or limited output is desired. Only one LM Parameter Line is allowed; this line must follow the Program Control Line and precede the RSS Control Line(s).

LM Parameter Line
Format(2F10.2,5X,5A1,9X,I1)

	Column	Format	Item	
1	1–10	F10.2	Tolerance for a match of the cell edges (Å)	
2	11–20	F10.2	Tolerance for a match of the cell volume (percentage of $Å^3$)	
	21–25	5X	Blank	
3	26–30	5A1	I/O/	Inorganic/Organic/ May specify one or more files to be searched.
	31–39	9X	Blank	
4	40	I1	Blank/1/	Print/Do not print/ RSS output

Notes:

1 Although the minimum tolerance allowed by the program is 0.02 Å, this value is NOT recommended for routine use. A tolerance of 0.10 Å is a more reasonable value to specify for most problems. The user may wish to increase this tolerance in a second run depending on the results obtained. It must be remembered that the known data in the search file(s) may not be as accurate and/or as precise as the experimental data input to the program.

2 Although the minimum tolerance allowed by the program is 5.0 percent, this value is NOT recommended for routine use. A tolerance of 10.0 percent is a more reasonable value to specify for most problems. The user may wish to increase this tolerance in a second run depending on the results obtained. It must be remembered that the known data in the search file(s) may not be as accurate and/or as precise as the experimental data input to the program.

3 One or more of the 1-line files may be searched in a single run. If no file is specified, the inorganic 1-line file will be searched.

4 In general, it is very useful to print the results of the reduction and derivative lattice calculations. However, when operating the program in a 'demand' environment or in cases where large numbers of derivative lattices are calculated, the user may wish to suppress this output.

c. RSS Control Line

The RSS Control Line defines the input lattice and the derivative lattices to be calculated. The lattice is defined by specifying the cell centering and all six unit cell parameters. The program will always carry out the cell reduction calculations. To calculate derivative lattices, it is necessary to tell the program whether to calculate supercells, subcells, or both supercells and subcells. In addition, for derivative lattice calculations, it is necessary to tell the program which multiples of the reduced cell volume (V) should be considered. Supercells having 2 to 9 times the volume of the reduced input cell and/or subcells having 1/2 to 1/9 times the volume of the reduced input cell may be calculated. There are 7 unique derivative lattices (supercells or subcells, respectively) having 2 or 1/2 times the volume of the reduced input cell, 13 derivative lattices with 3V or 1/3V, 35 with 4V or 1/4V, 31 with 5V or 1/5V, 91 with 6V or 1/6V, 57 with 7V or 1/7V, 155 with 8V or 1/8V, and 130 with 9V or 1/9V.

The RSS Control Line(s) must follow the Program Control Line and the LM Parameter Line. The number of RSS Control Lines must be equal to the number of problems specified on the Program Control Line.

RSS Control Line
Format(I1,2X,2I1,3X,2A1,6F10.2)

	Column	Format	Item
1	1	I1	Blank/1/2/3/ Blank = Reduction 1 = Reduction + supercells 2 = Reduction + subcells 3 = Reduction + supercells, subcells
	2–3	2X	Blank
2	4	I1	Blank/2/3/4/5/6/7/8/9/ Initial value (n1) to define the range of volumes for calculated derivative lattices.

3	5	I1	Blank/2/3/4/5/6/7/8/9/ Final value (n2) to define the range of volumes for calculated derivative lattices.
	6–8	3X	Blank
4	9	A1	P/A/B/C/F/I/R/ Cell centering
5	10	A1	R/H/ Rhombohedral/Hexagonal/ metric axes. Used only for rhombohedral lattices.
6	11–20	F10.2	a (Å)
7	21–30	F10.2	b
8	31–40	F10.2	c
9	41–50	F10.2	alpha (°)
10	51–60	F10.2	beta
11	61–70	F10.2	gamma

Notes:

1 If only a reduction is to be carried out, this field is left blank. If derivative lattices are to be calculated, then a 1, 2 or 3 is used for supercells, or subcells, or both supercells and subcells, respectively.

2 If only a reduction is to be carried out, this field is left blank. If derivative lattices are to be calculated, use an integer (n1) from 2 to 9.

3 If only a reduction is to be carried out, this field is left blank. If derivative lattices are to be calculated, use an integer (n2) from 2 to 9, but greater than or equal to n1.

2–3 These two integers (n1 and n2) are used to define the range of volumes for the derivative lattices to be calculated. The supercells to be calculated will have volumes ranging from (n1)V to (n2)V while the volumes for the subcells to be calculated will range from (1/n1)V to (1/n2)V. Especially when some chemical information is known, it is recommended to check routinely for the 55 supercells of 2,3, and 4 times the volume and the 55 subcells of 1/2,1/3, and 1/4 times the volume of the reduced input cell (i.e., n1 = 2, n2 = 4, with a '3' in column 1).

4 To define the lattice, both the cell and cell centering are required. A symbol specifying the cell centering must be placed in columns 9 and 10. A one character symbol is used for P,A,B,C,F, and I centered cells. For a cell defining a rhombohedral lattice, a two character symbol is required (RR or RH); the first character of this symbol ('R') is placed in column 9.

5 Column 10 is left blank unless the input cell defines a rhombohedral lattice. For a cell defining a rhombohedral lattice, an 'R' is placed in column 10 if the lattice is defined by a primitive rhombohedral cell (rhombohedral axes), or an 'H' is used if the lattice is defined by a triply primitive rhombohedral cell (metrically hexagonal axes).

6–8 Cell edges (Å).

9–11 Cell angles (°). Decimal numbers must be used for fractions of a degree. All six cell parameters must always be specified regardless of the crystal symmetry.

4. Examples of input flowstreams

a. Example 1

```
.........1.........1.........1.........1.........1.........1.........1

1   LM        3
2           0.10       10.0          OI
3             C 20.44      3.49       10.33      90.0       106.48     90.0
4             P 8.095      8.096      30.667     88.69      57.95      87.48
5   1  22     P 13.595     4.638      10.321     90.0       98.28      90.0
6   LM        1
7           0.10       10.0          O
8   1  22     P 13.595     4.638      10.321     90.0       98.28      90.0
```

Notes:

1 The 'LM ' in columns 1–5 indicates that the LM program function will be executed; the '3' in column 10 specifies that three independent problems are to be considered. This means that three RSS Control Lines must follow the Program Control Line and the LM Parameter Line.

2 The tolerance for a match of the cell edges (Å) is 0.10 (columns 1–10) while the tolerance for a match of the cell volume (Å^3) is 10.0 percent (columns 11–20). The 'OI' in columns 29–30 indicates that both the organic and inorganic data will be searched for a match of a,b,c,V. Since column 40 is blank, the results of the reduction and derivative lattice calculations will be printed.

3 Since column 1 is blank, the cell will be reduced and no derivative lattices will be calculated. Columns 4–5 are also left blank for reduction-only calculations. The 'C ' in columns 9–10 indicates that the input cell is C-centered. All six unit cell parameters are specified in columns 11–70.

4 This RSS Control Line directs the program to reduce a primitive cell.

5 The '1' in column 1 specifies that supercells of the lattice will be calculated. The '22' in columns 4–5 signify that the 7 unique supercells of twice the volume of the reduced input cell will be calculated. The 'P ' in columns 9–10 indicates that the input cell is primitive. All six unit cell parameters are specified in columns 11–70.

1–5 Although 3 independent problems are input to the LM program function, a total of 10 lattices (3 reduced input cells plus 7 reduced derivative supercells) are to be searched against the organic and inorganic data from the *NBS Crystal Data File*.

6 The LM program function is to be executed a second time with one independent problem to be considered. (This second operation will not be carried out by the program.)

7 This LM Parameter Line specifies that tolerances of 0.10 Å and 10.0 percent will be used to define a match of a,b,c, and V, the organic data will be searched, and the RSS output will be printed.

8 Same as 5.

b. Example 2

```
.........1.........1.........1.........1.........1.........1.........1

1   LM       4
2          0.10       10.0          I          1
3              P 3.0804     3.0806     15.122     89.96      89.99      119.99
4              C 6.282      15.203     5.674      90.0       114.04     90.0
5              P 5.674      6.282      8.225      67.55      81.05      65.96
6              P 7.751      7.393      7.395      63.93      72.22      103.27
```

Notes:

1 The 'LM ' in columns 1–5 indicates that the LM program function will be executed; the '4' in column 10 specifies that four independent problems are to be considered. This means that four RSS Control Lines must follow the Program Control Line and the LM Parameter Line.

2 Tolerances of 0.10 Å (columns 1–10) and 10.0 percent (columns 11–20) will be used to define a match of a,b,c,V. In this case, only the inorganic data will be searched. The '1' in column 40 indicates that the results of the reduction and derivative lattice calculations will not be printed.

3 Since column 1 is blank, the cell will be reduced and no derivative lattices will be calculated. Columns 4–5 are also left blank for reduction-only calculations. The 'P ' in columns 9–10 indicates that the input cell is primitive. All six unit cell parameters are specified in columns 11–70.

4 This RSS Control Line directs the program to reduce a C-centered cell.

5–6 Same as 3.

5. Examples of computer output

a. Example 1

The computer output following this section results from the input flowstream discussed above for Example 1 (sec. II.F.4.).

1. Page 1 of computer output

Since the results of the reduction and derivative lattice calculations are to be printed, a description of the RSS output parameters is given.

2. Pages 2–5 of computer output

There are three independent problems to be considered. Each of the input cells will be reduced and, if indicated, derivative supercells and/or subcells will be calculated. These reduced cells will be matched against data from the *NBS Crystal Data File*. See section III for a more detailed discussion of the RSS results.

The results of the reduction calculations for the first problem are given on the second page. This problem was discussed previously in section II.B. and the identification process was illustrated in figure 2.

The reduction output for the second independent problem is given on page 3. In this example, the input cell was determined on an automated diffractometer from a twinned crystal. When the input cell is reduced and the reduced cell matrix is analyzed, the orthorhombic nature of the lattice becomes apparent. The reduced form corresponds to number 13 in table 3 (sec. III). The matrix (1 1 0 / -1 1 0 / 0 0 1) will transform the reduced cell to a C-centered orthorhombic cell.

The input cell for the third independent problem is reduced and the seven supercells having twice the volume of the reduced cell are calculated. The output for these calculations is given on pages 4 and 5. The input cell was determined on an automated diffractometer. The structure solution was not completely successful as there appeared to be an unusual amount of disorder. A cell was determined a second time and it was found to have twice the volume. When the structure was solved on the basis of the new cell, the disorder disappeared. The third input cell is the subcell that was determined by missing nodes in reciprocal space. This example illustrates how a compound can be identified in spite of certain experimental errors by systematically calculating derivative lattices and searching the files of known compounds.

3. Page 6 of computer output

This page summarizes the data input to the lattice-matching procedure. First, a list of unknowns is given. The 'Original Sequence' column corresponds to the reduced cells and reduced derivative cells as they are calculated by the program. Thus, Original Sequence numbers 1, 2, and 3 correspond to the reduced cells for the first, second, and third independent problems, respectively. The Original Sequence numbers 4 through 10 correspond to the Supercells 1 through 7 given on pages 4 and 5 of the computer output. These lattices have been sorted according to the increasing values of the reduced cell parameters. The 'Search Sequence' corresponds to the order of the lattices after this sort has been completed. There are 10 unknown lattices to be searched against the file of known compounds. Tolerances of 0.10 Å and 10.0 percent will be used to define a match of a,b,c, and V.

4. Page 7 of computer output

The matches obtained when searching the inorganic data from the *NBS Crystal Data File* are presented here. This data is sorted according to the 'Original Sequence' of the input cells. Thus, the first independent problem (Original Sequence 1) was found to be sodium sesquicarbonate by a direct match of the reduced cell parameters. As explained in section II.B., this identification by lattice matching was confirmed by a full structure determination. The match of a,b,c,V for Original Sequence 3 is not valid since the cell was determined from an organic compound.

5. Page 8 of computer output

The matches obtained when searching the organic data from the *NBS Crystal Data File* are given on this page. The second independent problem (Original Sequence 2) was found to be potassium antimony tartrate hydrate by a direct match of the reduced cell parameters. There are no direct matches of the reduced cell parameters for the third independent problem. However, a lattice match was found for one of the supercells having twice the volume of the reduced input cell. The Original Sequence 5 corresponds to Supercell 2 in the RSS output. For both the second and third independent problems, the identification made by lattice matching was verified on the basis of the known chemistry.

6. Page 9 of computer output

Within a single computer run, the LM program function may be executed only once. This restriction is intended to discourage the inappropriate use of the LM program function. For example, if data for five organic compounds are to be analyzed, the user probably should not attempt five different searches. In general, since the LM program function employs a grouped-entry strategy, the most efficient method would be to include the data for all five organic compounds in a single computer run. In addition, the grouped-entry strategy enables the user to check routinely for matches of the reduced input cells as well as for calculated derivative cells.

b. Example 2

The computer output following this section results from the input flowstream discussed above for Example 2 (sec. II.F.4.).

1. Page 1 of computer output

Four independent problems are to be considered. The input cells will be reduced and matched against data from the *NBS Crystal Data File*. For this example, the results of the RSS calculations have not been printed.

2. Page 2 of computer output

This page summarizes the data input to the lattice-matching procedure. First, a list of unknowns is given. The 'Original Sequence' column corresponds to the reduced cells as they were calculated by the program. Thus, Original Sequence numbers 1,2,3, and 4 correspond to the reduced cells for the first, second, third, and fourth independent problems, respectively. These lattices have been sorted according to the increasing values of the reduced cell parameters. The 'Search Sequence' corresponds to the order of the lattices after this sort has been completed and duplicate lattices have been deleted. Duplicate lattices are defined as those having the same a,b,c within three decimal places and the same alpha, beta, gamma, within two decimal places. Duplicate lattices are not considered in the lattice-matching procedure for the sole purpose of eliminating repetitive output. There are several ways in which duplicate lattices can be input to the lattice-matching procedure. In this example, independent problems 2 and 3 reduced to the same cell. Another common way is through the generation of derivative supercells and/or subcells. For certain specialized triclinic lattices or for lattices having higher metric symmetry, some of the derivative lattices are metrically identical although they are oriented differently in space.

In summary, there are three unknown lattices to be searched against the file of known compounds. One duplicate lattice has been eliminated from the search procedure. Tolerances of 0.10 Å and 10.0 percent will be used to define a match of a,b,c, and V.

3. Page 3 of computer output

The matches obtained when searching the inorganic data are presented here. This data is sorted according to the 'Original Sequence' of the input cells.

The first independent problem (Original Sequence 1) was found to be silicon carbide. For this example, refined cell parameters were input to the program. When this cell is reduced, the resulting cell requires further reduction when the experimental error is considered. This example is discussed in detail in section III.B.4.b. In practice, two experimentally determined cells defining the same lattice will always give the same a,b,c (within experimental error) for the reduced cell, but in certain cases, the reduced cell angles may differ due to the interactions of the experimental errors with the normalization procedure and the process of satisfying the special conditions for reduction (for details, see sec. III). For this reason, the program matches only the cell edges and volume of the unknown reduced cell against the reduced cell file of known compounds. In this example, even though the cell angles are different for the reduced input cell and the known cell, it is apparent that the two cells define the same lattice and a transformation matrix relating them can be found by inspection. In more difficult cases, further reduction must be carried out (see sec. III) or a mathematical approach must be used to determine whether the two cells define the same lattice.

The second and third input cells were obtained using data from the same single crystal. As expected, these input cells reduced to the same cell. Since the third reduced cell was deleted from the search procedure, no computer output is expected. The second independent problem (Original Sequence 2) was identified as calcium sulfate dihydrate on the basis of the lattice and known chemical information.

There are nine matches of a,b,c,V for the fourth independent problem. Of these, two are direct cell matches. The identification of this unknown was made on the basis of the cell parameters and known chemical data. The unknown was deduced to be $Sr(ClO_3)_2 \cdot H_2O$ because it was isostructural with the barium analog in the *NBS Crystal Data File*. This example illustrates that every match of a,b,c,V does not necessarily define the same lattice. When a mathematical procedure (Santoro, Mighell & Rodgers, 1980) is used, it can be shown that only the two direct cell matches define the same lattice as the input cell, the remaining seven matches of a,b,c,V do not. In the next version of the *NBS*LATTICE* program, this mathematical technique will be added to distinguish between lattices that have only a,b,c,V in common and lattices that are identical. At present, knowledge of the empirical formula or some other chemical information is almost always sufficient to eliminate unwanted matches.

Example 1
Section II.F.5.a.
Page 1

*** NBS*LATTICE ***

A PROGRAM TO ANALYZE LATTICE RELATIONSHIPS
Version of Spring, 1985

NBS Crystal Data Center
National Bureau of Standards
Reactor Radiation Division
Gaithersburg, MD 20899

** REDUCTION AND DERIVATIVE LATTICE **

These calculations fall into two categories:

I. Reduction of an input cell.

CELL 1 = Input cell. This cell may be primitive or centered (A,B,C,I,F,RR,RH).
CELL 2 = Reduced primitive cell of the lattice.
T 1 = A matrix that transforms CELL 1 to a primitive cell of the lattice.
T 2 = A matrix that transforms CELL 1 to CELL 2.

II. Calculation and reduction of a series of derivative supercells and/or subcells. These derivative cells are calculated from the reduced cell of the lattice (i.e. to carry out the Type II calculation, the program first carries out the Type I calculation).

CELL 1 = Reduced primitive cell (i.e. CELL 2 from Part I).
CELL 2 = Reduced supercell or subcell.
T 1 = A matrix that transforms CELL 1 to a supercell or subcell of the lattice.
T 2 = A matrix that transforms CELL 1 to CELL 2.

For CELL 1 and CELL 2, the output parameters given are: a, b, c, alpha, beta, gamma and volume. Cell edges are in angstroms and angles in degrees.

The reduced cell matrix is of the form:

a.a	b.b	c.c
b.c	a.c	a.b

.

Page 2

REDUCTION AND DERIVATIVE LATTICE

Number of independent problems to study = 3

Lattice Matching of reduced cell(s) with the
NBS Crystal Data File

1. REDUCTION

** Initial Cell is C-Centered **

T 1=	.50	-.50	.00/	.50	.50	.00/	.00	.00	1.00
T 2=	.00	1.00	.00/	.00	.00	1.00/	.50	-.50	.00
T 2 INV=	1.00	.00	2.00/	1.00	.00	.00/	.00	1.00	.00

** Cell Matrix **

CELL 1=	20.4400	3.4900	10.3300	90.000	106.480	90.000	V1=	706.62	12.180	106.709	107.493
CELL 2=	3.4900	10.3300	10.3679	106.238	99.689	90.000	V2=	353.31	-29.949	-6.090	.000

Page 3

2. REDUCTION

** Initial Cell is Primitive **

```
T 1=       1.00    .00    .00/    .00   1.00    .00/    .00    .00   1.00
T 2=       1.00    .00    .00/    .00  -1.00    .00/   2.00    .00  -1.00
T 2 INV=   1.00    .00    .00/    .00  -1.00    .00/   2.00    .00  -1.00
```

** Cell Matrix **

```
CELL  1=    8.0950    8.0960   30.6670     88.690    57.950    87.480     V1=   1701.85      65.529    65.545   675.638
CELL  2=    8.0950    8.0960   25.9930     90.024    90.185    92.520     V2=   1701.85       -.087     -.678    -2.882
```

Page 4

3. SUPERLATTICES

** Initial Cell is Primitive **

```
T 1=       1.00    .00    .00/    .00   1.00    .00/    .00    .00   1.00
T 2=        .00   1.00    .00/    .00    .00  -1.00/  -1.00    .00    .00
T 2 INV=    .00    .00  -1.00/   1.00    .00    .00/    .00  -1.00    .00
```

** Cell Matrix **

```
CELL  1=   13.5950    4.6380   10.3210     90.000    98.280    90.000     V1=    643.99      21.511   106.523   184.824
CELL  2=    4.6380   10.3210   13.5950     98.280    90.000    90.000     V2=    643.99     -20.207      .000      .000
```

Superlattices for Delta = 2

***** Supercell 1 *****

```
T 1=       1.00    .00    .00/    .00   1.00    .00/    .00    .00   2.00
T 2=       1.00    .00    .00/    .00   1.00    .00/    .00    .00   2.00
T 2 INV=   1.00    .00    .00/    .00   1.00    .00/    .00    .00    .50
```

** Cell Matrix **

```
CELL  1=    4.6380   10.3210   13.5950     98.280    90.000    90.000     V1=    643.99      21.511   106.523   739.296
CELL  2=    4.6380   10.3210   27.1900     98.280    90.000    90.000     V2=   1287.99     -40.413      .000      .000
```

***** Supercell 2 *****

```
T 1=       1.00    .00    .00/    .00   1.00   1.00/    .00    .00   2.00
T 2=      -1.00    .00    .00/    .00  -1.00  -1.00/    .00  -1.00   1.00
T 2 INV=  -1.00    .00    .00/    .00   -.50   -.50/    .00   -.50    .50
```

** Cell Matrix **

```
CELL  1=    4.6380   10.3210   13.5950     98.280    90.000    90.000     V1=    643.99      21.511   250.934   331.761
CELL  2=    4.6380   15.8409   18.2143    105.746    90.000    90.000     V2=   1287.99     -78.301      .000      .000
```

```
                              ***** Supercell   3 *****

T 1=       1.00    .00   1.00/    .00   1.00    .00/    .00    .00   2.00
T 2=       2.00    .00    .00/    .00   1.00    .00/  -1.00    .00   1.00
T 2 INV=    .50    .00    .00/    .00   1.00    .00/    .50    .00   1.00                    ** Cell Matrix **

CELL  1=    4.6380   10.3210   13.5950     98.280    90.000    90.000          V1=   643.99      86.044   106.523   206.335
CELL  2=    9.2760   10.3210   14.3644     97.834   108.837    90.000          V2=  1287.99     -20.207   -43.022      .000


                              ***** Supercell   4 *****

T 1=       1.00    .00   1.00/    .00   1.00   1.00/    .00    .00   2.00
T 2=      -2.00    .00    .00/  -1.00  -1.00    .00/  -1.00    .00   1.00
T 2 INV=   -.50    .00    .00/    .50  -1.00    .00/   -.50    .00   1.00                    ** Cell Matrix **
```

Page 5

```
CELL  1=    4.6380   10.3210   13.5950     98.280    90.000    90.000          V1=   643.99      86.044   128.034   206.335
CELL  2=    9.2760   11.3152   14.3644     75.128    71.163    65.802          V2=  1287.99      41.718    43.022    43.022


                              ***** Supercell   5 *****

T 1=       1.00    .00    .00/    .00   2.00    .00/    .00    .00   1.00
T 2=      -1.00    .00    .00/    .00    .00  -1.00/    .00  -2.00    .00
T 2 INV=  -1.00    .00    .00/    .00    .00   -.50/    .00  -1.00    .00                    ** Cell Matrix **

CELL  1=    4.6380   10.3210   13.5950     98.280    90.000    90.000          V1=   643.99      21.511   184.824   426.092
CELL  2=    4.6380   13.5950   20.6420     98.280    90.000    90.000          V2=  1287.99     -40.413      .000      .000


                              ***** Supercell   6 *****

T 1=       1.00   1.00    .00/    .00   2.00    .00/    .00    .00   1.00
T 2=       2.00    .00    .00/  -1.00   1.00    .00/    .00    .00   1.00
T 2 INV=    .50    .00    .00/    .50   1.00    .00/    .00    .00   1.00                    ** Cell Matrix **

CELL  1=    4.6380   10.3210   13.5950     98.280    90.000    90.000          V1=   643.99      86.044   128.034   184.824
CELL  2=    9.2760   11.3152   13.5950     97.548    90.000   114.198          V2=  1287.99     -20.207      .000   -43.022


                              ***** Supercell   7 *****

T 1=       2.00    .00    .00/    .00   1.00    .00/    .00    .00   1.00
T 2=       2.00    .00    .00/    .00   1.00    .00/    .00    .00   1.00
T 2 INV=    .50    .00    .00/    .00   1.00    .00/    .00    .00   1.00                    ** Cell Matrix **

CELL  1=    4.6380   10.3210   13.5950     98.280    90.000    90.000          V1=   643.99      86.044   106.523   184.824
CELL  2=    9.2760   10.3210   13.5950     98.280    90.000    90.000          V2=  1287.99     -20.207      .000      .000
```

Page 6

** LATTICE MATCHING **

Identification of unknown lattices using data from
the National Bureau of Standards Crystal Data File

*** UNKNOWNS ***

Search Sequence	Original Sequence	a	b	c	Alpha	Beta	Gamma	Vol
1	1	3.49000	10.33000	10.36790	106.23835	99.68945	90.00000	353.31
2	3	4.63800	10.32100	13.59500	98.28000	90.00000	90.00000	643.99
3	4	4.63800	10.32100	27.19000	98.28000	90.00000	90.00000	1287.99
4	8	4.63800	13.59500	20.64200	98.28000	90.00000	90.00000	1287.99
5	5	4.63800	15.84088	18.21429	105.74631	90.00000	90.00000	1287.99
6	2	8.09500	8.09600	25.99303	90.02367	90.18455	92.52000	1701.85
7	10	9.27600	10.32100	13.59500	98.28000	90.00000	90.00000	1287.99
8	6	9.27600	10.32100	14.36437	97.83365	108.83732	90.00000	1287.99
9	9	9.27600	11.31521	13.59500	97.54803	90.00000	114.19796	1287.99
10	7	9.27600	11.31521	14.36437	75.12755	71.16268	65.80204	1287.99

Original number of unknowns = 10
Number of duplicate unknowns = 0
Number of unknowns for search = 10

Tolerance for cell edges = .10
Tolerance for cell volume = 10.00

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INORGANIC
*** RESULTS ***

Search Sequence	Original Sequence	a	b	c	Alpha	Beta	Gamma	Vol
1	1	3.490	10.330	10.368	106.24	99.69	90.00	353.3

3.49 10.31 10.35 106.1 99.7 90.0 352 15 MT 2180 ACCRA9 2 167 1949 Na3 H (C O3)2 !2 H2 O

2	3	4.638	10.321	13.595	98.28	90.00	90.00	644.0

4.74 10.27 13.68 100.8 90.0 90.0 654 14 ML 9172 PRLAAZ 117 517 1928 Mg9 (O H , F)2 (Si O4)4

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ORGANIC
*** RESULTS ***

Search Sequence	Original Sequence	a	b	c	Alpha	Beta	Gamma	Vol	
6	2	8.095	8.096	25.993	90.02	90.18	92.52	1701.9	
8.09	8.09 25.93	90.0	90.0	92.5	1697	20 OT 15513	ICHAA3	8 209 1974	C8 H4 O12 Sb2 -2 !2 (K +) !3 (H2 O)
8.12	8.12 25.96	90.0	90.0	92.7	1708	20 OT 15653	KHTPAT	17 502 1966	C8 H4 O12 Sb2 -2 !2 (K +) !3 (H2 O)
5	5	4.638	15.841	18.214	105.75	90.00	90.00	1288.0	
4.62	15.93 18.27	105.6	90.0	90.0	1296	14 MT 1348	JACSAT	101 5858 1979	C12 H6 Cl2 I N O3
4.62	15.93 18.27	105.6	90.0	90.0	1296	14 MT 1349	ACBCAR	36 2819 1980	C12 H6 Cl2 I N O3

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INPUT ERROR ... Only one Lattice Matching operation per run is allowed.

Example 2
Section II.F.5.b.
Page 1

*** NBS*LATTICE ***

A PROGRAM TO ANALYZE LATTICE RELATIONSHIPS
Version of Spring, 1985

NBS Crystal Data Center
National Bureau of Standards
Reactor Radiation Division
Gaithersburg, MD 20899

REDUCTION AND DERIVATIVE LATTICE

Number of independent problems to study = 4

Lattice Matching of reduced cell(s) with the
NBS Crystal Data File

Page 2

** LATTICE MATCHING **

Identification of unknown lattices using data from
the National Bureau of Standards Crystal Data File

*** UNKNOWNS ***

Search Sequence	Original Sequence	a	b	c	Alpha	Beta	Gamma	Vol
1	1	3.08097	3.08060	15.12200	89.96000	89.95000	59.99178	124.29
2	2	5.67400	6.28200	8.22488	67.54920	81.05002	65.96000	247.45
Delete	3	5.67400	6.28200	8.22500	67.55000	81.05000	65.96000	247.45
3	4	7.39300	7.39500	7.74953	103.27236	107.76093	116.07000	328.06

Original number of unknowns = 4
Number of duplicate unknowns = 1
Number of unknowns for search = 3

Tolerance for cell edges = .10
Tolerance for cell volume = 10.00

INORGANIC
*** RESULTS ***

Search Sequence	Original Sequence	a	b	c	Alpha	Beta	Gamma	Vol	
1	1	3.081	3.081	15.122	89.96	89.95	59.99	124.3	
3.08	3.08 15.11	90.0	90.0 120.0	124 186 HT	1000 BJAPAJ	1 174 1950 Si C			
2	2	5.674	6.282	8.225	67.55	81.05	65.96	247.5	
5.61	6.19 8.17	67.7	80.6 64.7	237	MN 14167 MIASA6	30 211 1953 (Y , Er) P O4 !2 H2 O			
5.67	6.28 8.20	67.4	80.9 65.8	246 15	MT 14467 IECHAD	28 441 1936 Ca S O4 !2 H2 O			
3	4	7.393	7.395	7.750	103.27	107.76	116.07	328.1	
7.30	7.30 7.78	117.9	117.9 90.0	310 140	TL 20605 ZAACAB	339 52 1965 Ba3 (Co O4) O			
7.31	7.31 7.69	90.0	90.0 120.0	355	HN 20640 BSCFAS	4805 1968 Tl0.33 (W0.67 Nb0.33) O3			
7.32	7.32 7.68	90.0	90.0 120.0	356	HN 20692 INOCAJ	5 1559 1966 Mo Rb0.27 O3			
7.32	7.32 7.80	117.9	117.9 90.0	312 140	TL 20693 ZAACAB	339 52 1965 Ba3 (Cr O4) O			
7.32	7.32 7.83	117.8	117.8 90.0	315 140	TL 20694 ZAACAB	339 52 1965 Ba3 (Fe O4) O			
7.34	7.34 7.77	118.1	118.1 90.0	311 140	TL 20793 ZAACAB	339 52 1965 Ba3 (Ge O4) O			
7.35	7.35 7.69	103.2	107.9 116.0	322 15	MT 20833 ACCRA9	5 845 1952 Ba (Cl O3)2 ! H2 O			
7.36	7.36 7.72	61.6	61.6 60.0	302 166	RN 20863 ZAACAB	357 264 1968 K2 Pt4 Se6			
7.40	7.40 7.75	103.1	107.9 116.1	328 15	MT 21025 JCPSA6	48 1883 1968 Ba (Cl O3)2 ! H2 O			

III. Reduction and derivative supercell and subcell calculations

A. Introduction

The reduction and derivative supercell and subcell program function carries out two types of calculations: 1) the calculation of the reduced cell of the lattice; and 2) the calculation and reduction of specified derivative supercells and/or subcells. Starting with any primitive or centered cell of the lattice, this program function calculates the standard cells which are useful in the determination of metric symmetry, in finding the relationships between unit cells, and in the characterization and identification of unknown materials.

B. Reduction

1. Theory and computer algorithm

The reduced cell (Niggli, 1928) is defined as a unique, primitive cell that is based on the three shortest noncoplanar vectors of the lattice and satisfies a specified set of mathematical conditions. For a cell to be reduced, the cell must be in normal representation and both the main and the special conditions for reduction must be satisfied. These conditions are given in table 1. The main conditions assure that one has a cell based on the three shortest lattice translations, while the special conditions assure that the cell is unique. It has been shown that in some lattices more than one cell is based on the three shortest lattice translations (Santoro & Mighell, 1970); Gruber (1973) has shown that at most five different cells of this type may exist in the same lattice.

A summary of the reduction procedure is outlined in figure 1. The computer program calculates the reduced cell starting with any primitive or centered cell of the lattice. To obtain the reduced cell, the program carries out a series of cell transformations. The total transformation matrix from the initial to reduced cell, T_t, is obtained by multiplying together the individual matrices in reverse order:

$$T_t = (T_n)\,(T_{n-1})\,(T_{n-2}) \ldots (T_1),$$

where T_n is the matrix used in the last cell transformation. If the initial cell is a primitive cell of the lattice, the transformation matrix, T_t, will have all integer elements and a determinant of one.

Reduction is a mathematical procedure that leads to a unique cell in all cases, provided there is no experimental error in the unit cell parameters. Unfortunately, experimental error is always present for cells determined in the laboratory. Furthermore, in our experimental work and in evaluating data for the NBS Crystal Data Center, we have noted that the reported precision on the unit cell parameters is not necessarily a reliable indicator of the accuracy, and that it would be dangerous to estimate accuracy from the reported precision in all cases. Therefore, when testing the conditions given in table 1, the present program does not use the reported experimental errors, but instead decides whether the conditions are satisfied to within standard tolerances fixed in the program. These standard tolerances are set low with respect to routinely reported estimated standard deviations (e.s.d.'s). The computer program reduces the cell based on its geometry and does not, in general, evaluate the effects of experimental errors in the reduction procedure. Therefore, certain precautions must be taken when interpreting the results of the reduction program; these are discussed in the following sections. Additional details concerning the reduction procedure used in the program are given in Acta Crystallographica (Santoro & Mighell, 1970), and in the *International Tables for X-ray Crystallography* (1969 *a*).

2. Uses of reduced cells

Since it is unique, the reduced cell has many practical applications. For example, the reduced cell can be used in the characterization and identification of materials. By transforming two different cells of the lattice to the same, standard cell, reduction procedures provide a straightforward means of relating different experimental data for a compound. In a similar manner, experience in the NBS Crystal Data Center has shown that the reduced cell plus some chemical information, such as the empirical formula, can be used to identify unknown materials. In fact, for most molecular compounds, the reduced cell alone is sufficient to identify the material. This identification procedure is based on matching the unknown reduced cell against the entire *NBS Crystal Data File* (1982). This File contains chemical and crystallographic data on approximately 60,000

materials; each lattice in the File is represented by its reduced cell. File surveys have shown that the lattice is highly characteristic of a material. This is not entirely surprising since matching reduced cell parameters may be thought of as matching the positions of all possible d-spacings of a powder pattern. The powder method of identification, based on matching observed d-spacings and intensities, is a widely used analytical technique. However, there are many advantages to the lattice-matching approach. Additional information concerning the lattice-formula identification procedure is given in section II.

In addition to identification, the reduced cell may be used to determine the metric symmetry of the lattice. Table 3 defines the relationships between the 44 reduced forms, calculated from the reduced cell, and the conventional Bravais lattice types. Analyses of the reduced cells in the *NBS Crystal Data File* have shown that the metric symmetry and the crystal symmetry are usually identical. When the two symmetries differ, it is not uncommon for the crystal symmetry to have been reported incorrectly in the literature. For details concerning metric symmetry determination using the reduced cell, see *International Tables for X-ray Crystallography* (1969 a), and Mighell & Rodgers (1980).

3. Interpreting the results of a reduction program

For each unit cell, the computer program always gives the unique, reduced cell defined by Niggli (1928). However, in certain cases, after the experimental error has been considered, further reduction may be necessary. This is due to the interactions of the experimental errors with the normalization procedure and the process of satisfying the special conditions for reduction. Therefore, after the reduced cell and reduced form have been calculated, one should assume liberal experimental errors and inspect the conditions given in table 1. If there is additional specialization in the reduced form (i.e., $b \cdot c = 0$, $a \cdot b = 1/2a \cdot a$, etc.), further reduction may be possible. Table 2 gives a procedure for determining the reduced cell from an unreduced cell based on the three shortest lattice translations. For cases in which further reduction may be possible, an alternate procedure may be used. First, when inspecting table 1, look for extra specialization in the reduced form and set the dot products to the ideal values; re-calculate the 'reduced' cell from the idealized reduced form. Second, re-run the reduction program using the idealized 'reduced' cell. Third, check the new reduced form using tables 1, 2 and 3 to see that the reduction process is complete and that the new cell reveals the highest possible metric symmetry. Finally, apply the transformation matrix to the initial cell and evaluate the experimental errors.

In the determination of metric symmetry, the special conditions for reduction are critical and care must be taken to assure that the reduced cell revealing the highest metric symmetry has been obtained. Therefore, after the reduced form has been calculated, liberal experimental errors should be used when inspecting tables 1, 2, and 3. Any extra specialization in the cell matrix (see table 1) may mean that further reduction is possible and that the reduced form does not reveal the highest metric symmetry. Alternatively, we have found that a matrix technique (Himes & Mighell, 1982) is extremely reliable in determining the metric symmetry of the lattice to within any specified tolerances for the unit cell parameters. The matrix technique can be used independently or in conjunction with reduction. In addition to symmetry determination, it provides a straightforward method to adjust the experimentally determined cell parameters so that one can calculate the 'ideal' reduced cell and reduced form (Himes, 1983). Clegg (1981) and Le Page (1982) provide alternative procedures for obtaining a cell that reveals the highest metric symmetry of the lattice.

When identifying an unknown using the reduced cell, it has been found that the three shortest vectors and cell volume are usually sufficient to make the identification. In practice, a match of a,b,c,V of the unknown reduced cell against an entry in the *NBS Crystal Data File* can be made with the angles of the two cells in disagreement. It is still likely that the two cells define the same lattice because, when the experimental errors are considered, one of the cells may not be normalized or may not be reduced with respect to the special conditions. Sometimes it is obvious that the two cells define the same lattice and the transformation matrix relating them can be found by inspection. In more difficult cases, further reduction must be carried out, or a mathematical approach (Santoro, Mighell & Rodgers, 1980) may be used in order to determine if the two cells define the same lattice.

In summary, the computer program always calculates the reduced cell based on the geometry of the input cell. When the reduced cell and reduced cell matrix are evaluated using liberal experimental errors, in certain cases, further reduction may be indicated. In practice, the reduction program almost always obtains the reduced cell, or a cell whose reduced form has one or more unsymmetrical scalars near zero and requires re-normalization (see table 2) to obtain the reduced form revealing the highest possible symmetry of the lattice. Other instances in which further reduction is necessary are exceptional.

4. Examples of interpreting the results of a reduction program

a. Further reduction is not necessary

The compound dichlorobis(4-vinylpyridine)zinc(II) has been described in the triclinic space group P1 with the unit cell parameters

a = 7.501(4)	b = 7.522(5)	c = 14.482(6) Å
α = 90.41(4)	β = 90.53(4)	γ = 105.29(5)°

(Steffen & Palenik, 1977; see also Marsh & Schomaker, 1979). In this case, the published unit cell is the reduced cell. Inspection of the following reduced cell matrix reveals that $a \cdot a = b \cdot b$ and $b \cdot c = a \cdot c$ within a small tolerance.

$$\begin{pmatrix} 56.265 & 56.580 & 209.728 \\ -.780 & -1.005 & -14.879 \end{pmatrix}$$

According to table 1, all of the main and special conditions for a type II cell are still satisfied if these equalities are true. Thus, further reduction is not indicated and it is not necessary to consult table 2. The specialized reduced cell matrix corresponds to reduced form number 14 in table 3. The matrix (1 1 0 / -1 1 0 / 0 0 1) may be used to transform the reduced cell to the C-centered monoclinic cell with

a = 9.115	b = 11.942	c = 14.482 Å
α = 89.93	β = 90.77	γ = 89.83° .

If more liberal tolerances are assumed, the reduced cell matrix is even more specialized with $a \cdot a = b \cdot b$ and $b \cdot c = a \cdot c = 0$. With these extra conditions, no further reduction is necessary (see table 1) and the reduced form corresponds to number 13 in table 3. The reduced cell can be transformed to a C-centered orthorhombic cell with the same cell parameters as the C-centered monoclinic cell. Thus, even though the interpretation of the unit cell parameter errors does not result in further reduction, it does affect the analysis of the metric symmetry for this compound. If a value of 0.04 degrees, obtained from the original triclinic cell, is used to estimate the errors for the angles of the transformed cells, the compound will have exact monoclinic metric symmetry within approximately 5 e.s.d.'s and exact orthorhombic metric symmetry within approximately 20 e.s.d.'s. To summarize, we first assumed liberal experimental errors and looked for specialization in the reduced cell matrix. Then, the conditions for reduction specified in table 1 were checked. In this example, the conditions were met. If all of the conditions were not satisfied due to the additional specialization, table 2 could be used to obtain the appropriate transformation matrix to the reduced cell. Finally, table 3 was used for the determination of metric symmetry.

An alternate approach that could be used is to look for specialization in the reduced cell matrix and set the dot products to the ideal values. Idealized cell parameters are then calculated from the idealized cell matrix. Table 1 must be checked to verify that the idealized cell is reduced; if not, table 2 may be used or the idealized cell may be rerun through the reduction program. Finally, table 3 is used to determine the metric symmetry of the idealized reduced cell.

Data for the Zn(II) compound will be used to illustrate the second approach. For the Zn(II) compound to have monoclinic metric symmetry, it was assumed that the reduced cell matrix was specialized with $a \cdot a = b \cdot b$ and $b \cdot c = a \cdot c$. One way to idealize the reduced cell matrix is to take the average of the appropriate dot products. Thus, the idealized cell matrix becomes

$$\begin{pmatrix} 56.423 & 56.423 & 209.728 \\ -.892 & -.892 & -14.879 \end{pmatrix}$$

and the idealized cell parameters are

a = 7.5115	b = 7.5115	c = 14.482 Å
α = 90.47	β = 90.47	γ = 105.29 °.

For the compound to have orthorhombic metric symmetry, the reduced cell matrix must be specialized so that $a \cdot a = b \cdot b$ and $b \cdot c = a \cdot c = 0$. The idealized cell matrix becomes

$$\begin{pmatrix} 56.423 & 56.423 & 209.728 \\ 0 & 0 & -14.879 \end{pmatrix}$$

and the idealized cell parameters are

$a = 7.5115$	$b = 7.5115$	$c = 14.482$ Å
$\alpha = 90.00$	$\beta = 90.00$	$\gamma = 105.29$ °.

When table 1 is checked or the idealized cell parameters are rerun through the reduction program, it can be shown that, in this example, both the idealized monoclinic and the idealized orthorhombic cells are also the idealized reduced cells. (This is not always true.) Since the original triclinic cell was the reduced cell, the reported e.s.d.'s may be applied directly to the idealized reduced cells when estimating the deviations from exact monoclinic or orthorhombic metric symmetry. The Zn(II) compound is metrically monoclinic since the experimental errors estimated in this way correspond to a maximum of approximately 3 e.s.d.'s. In order to have exact orthorhombic metric symmetry, the original triclinic cell parameters must be changed by a maximum of approximately 13 e.s.d.'s.

Although these two analyses of the reduced cell matrix were very similar, the estimate of the number of e.s.d.'s required for exact monoclinic or orthorhombic metric symmetry varied. In general, there are several ways to analyze the reduced cell matrices when considering the effects of the experimental errors. It should be remembered that the method chosen may not be the one that minimizes the estimated errors. Therefore, all results should be considered even if they require relatively large experimental errors. In this example, experimental techniques should be used to determine whether the Zn(II) compound has triclinic, monoclinic or orthorhombic crystal symmetry.

b. Further reduction is required due to a normalization problem

The *NBS*LATTICE* program always calculates the reduced cell based on the geometry of the input cell. In the previous example, the cell obtained from the reduction program did not require further reduction when rather large experimental errors were assumed. However, as this example illustrates, the experimental error need not be large to interact with the normalization requirements and the special conditions for reduction. It is important to remember that the tolerances for testing the conditions given in table 1 are set low with respect to routinely reported e.s.d.'s.

The unit cell parameters,

$a = 3.0804(6)$	$b = 3.0806(8)$	$c = 15.122(4)$ Å
$\alpha = 89.96(2)$	$\beta = 89.99(2)$	$\gamma = 119.99(2)$ °,

were determined for alpha-silicon carbide using an automated diffractometer. The following reduced cell and reduced cell matrix were calculated by the program:

reduced cell:	$a = 3.0810$	$b = 3.0806$	$c = 15.122$ Å
	$\alpha = 89.96$	$\beta = 89.95$	$\gamma = 59.99$ °

reduced cell matrix = $\begin{pmatrix} 9.492 & 9.490 & 228.675 \\ .033 & .041 & 4.747 \end{pmatrix}$.

Inspection of the reduced cell matrix reveals that it is specialized with $a \cdot a = b \cdot b = 2a \cdot b$ and $b \cdot c = a \cdot c = 0$ within a small tolerance. When table 1 is checked, all of the main and special conditions for a positive reduced form are satisfied. However, the cell is NOT reduced because it is neither a type I nor a type II cell when the extra specialization is introduced. This is apparent when the idealized cell parameters are calculated from the idealized cell matrix.

Idealized cell matrix = $\begin{pmatrix} 9.492 & 9.492 & 228.675 \\ 0 & 0 & 4.746 \end{pmatrix}$

Idealized cell:	$a = 3.0809$	$b = 3.0809$	$c = 15.122$ Å
	$\alpha = 90.00$	$\beta = 90.00$	$\gamma = 60.00$ °

The computer program calculated the geometrically reduced cell with all angles less than 90 degrees (type I cell). However, when small experimental errors are assumed, further reduction is indicated. Before using table 2 to find a matrix from the unreduced to the reduced cell, one must recognize that the cell type is 'non-standard' because the angles are neither all less than 90 degrees (type I) nor all greater than or equal to 90 degrees (type II). The special relations between the unsymmetrical scalars can be found in the fifth row of table 2, non-standard condition (d), with $b \cdot c = 0$, $a \cdot c = 0$ and $a \cdot b > 0$. Using the table, the new cell matrix (idealized) becomes

$$\begin{pmatrix} 9.492 & 9.492 & 228.675 \\ 0 & 0 & -4.746 \end{pmatrix}.$$

At this point, reduction is complete. The resulting unit cell corresponds to a type II cell and all of the main and special conditions for a negative reduced form have been satisfied (table 1). This reduced form, number 12 in table 3, reveals the hexagonal symmetry of the lattice. The matrix (1 1 0 / 0 1 0 / 0 0 1) from the initial to the 'reduced' cell (calculated by the program) may be multiplied by the matrix (-1 0 0 / 0 1 0 / 0 0 -1) obtained from table 2 to obtain a transformation matrix (-1 -1 0 / 0 1 0 / 0 0 -1) from the initial cell to the reduced cell after allowing for the experimental errors.

The reduced cell calculated from the refined unit cell parameters had the a-cell parameter slightly greater than the b-cell parameter. This occurred because they were equal within the small tolerance set in the computer program. However, within the program, angles in the approximate range of 89.98 to 90.02 degrees are considered to be equal to 90 degrees. Since the value of alpha (89.96 degrees) was slightly outside of this range, a reduced cell requiring further reduction resulted. If the initial value for alpha were not 89.96 but 89.981, the reduced cell calculated by the program would require no further reduction. In this example, the need for further reduction arose because one or more of the unsymmetrical scalars was near zero. When these scalars are idealized to be zero, the cell matrix and, consequently, the unit cell are both non-standard. In practice, when considering the effects of experimental errors, the most common reason for a cell reduced by the computer program to require further reduction is this 'normalization' problem.

c. Example requiring further reduction

This example (Himes, 1983) shows that one must carefully inspect the relationships between the scalars in the reduced cell matrix output by a reduction program. Consider the reduced cell and reduced cell matrix calculated from a C-centered monoclinic cell (a = 18.21(1), b = 10.509(1), c = 20.69(1)Å, β = 126.00(5)°) reported in the literature.

Reduced cell:	a = 10.509	b = 10.512	c = 17.798 Å
	α = 107.12	β = 90.00	γ = 119.99 °

$$\text{Reduced cell matrix} = \begin{pmatrix} 110.44 & 110.55 & 316.77 \\ -55.07 & 0 & -55.22 \end{pmatrix}$$

With no experimental error, the cell is reduced and the reduced cell matrix corresponds to monoclinic reduced form number 39. However, within a small tolerance, the cell matrix is specialized so that $a \cdot a = b \cdot b$ and $|b \cdot c| = |a \cdot b| = a \cdot a/2$. Inspection of table 1 reveals that the cell is not reduced when these conditions are true. A transformation matrix to the reduced cell obtained after considering the effects of experimental error may be found by consulting table 2. First, the idealized cell matrix and cell are calculated.

$$\text{Idealized cell matrix} = \begin{pmatrix} 110.48 & 110.48 & 316.77 \\ -55.24 & 0 & -55.24 \end{pmatrix}$$

Idealized cell:	a = 10.51	b = 10.51	c = 17.80 Å
	α = 107.17	β = 90.00	γ = 120.00 °

Using this idealized cell matrix and table 2, the reduction can be completed in two steps. The idealized cell is a type II cell. The special relations between the scalars, $a \cdot a = b \cdot b$ and $|a \cdot c| < |b \cdot c|$, are found in the seventh row of the table. The transformation matrix (0 -1 0 / -1 0 0 / 0 0 -1) is to be applied to the cell, and the idealized cell matrix becomes:

$$\begin{pmatrix} 110.48 & 110.48 & 316.77 \\ 0 & -55.24 & -55.24 \end{pmatrix}.$$

According to table 1, special conditions (d) and (e) for a type II cell are not satisfied; thus, further reduction is necessary. In this case, the special relations between the scalars can be found in row 13 for a type II cell with $a \cdot c = -a \cdot a/2$ and $a \cdot b \neq 0$. The transformation matrix to be applied to the cell is (-1 0 0 / 0 1 0 / -1 0 -1) and the idealized cell matrix becomes:

$$\begin{pmatrix} 110.48 & 110.48 & 316.77 \\ 55.24 & 55.24 & 55.24 \end{pmatrix}.$$

The conditions for a positive reduced form (calculated from a type I cell) now apply. Inspection of table 1 reveals that the reduction process has been completed. The idealized reduced cell, with

$$\begin{array}{lll} a = 10.51 & b = 10.51 & c = 17.80\ \text{Å} \\ \alpha = 72.83 & \beta = 72.83 & \gamma = 60.00^\circ, \end{array}$$

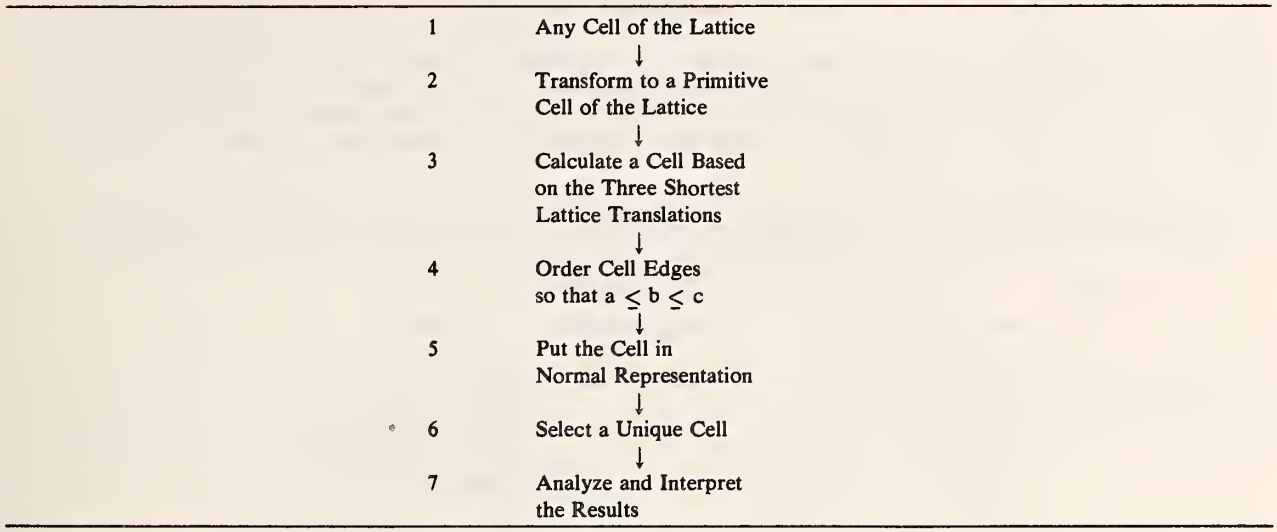
may be calculated from the idealized reduced cell matrix. The reduced form, number 9 in table 3, reveals the rhombohedral nature of the lattice.

A transformation matrix from the initial cell to the reduced cell may be obtained by multiplying together the transformation matrix output by the computer program (0 1 0 / -.5 -.5 0 / 1 0 1) and the two matrices obtained from table 2. Thus, the matrix (-.5 -.5 0 / 0 -1 0 / .5 -.5 1) may be used to transform the C-centered monoclinic cell to the 'non-idealized' reduced cell with

$$\begin{array}{lll} a = 10.512 & b = 10.509 & c = 17.808\ \text{Å} \\ \alpha = 72.84 & \beta = 72.78 & \gamma = 60.01^\circ. \end{array}$$

An alternate procedure would be to idealize the initial cell matrix output by the computer program, calculate the idealized cell, and input this cell into the reduction program. In either case, a transformation matrix to the 'non-idealized' reduced cell (after the consideration of the experimental error) can be found.

Figure 1. *Reduction sequence*



Notes:

1 The program reads in the cell and cell centering.

2 If other than primitive, the program transforms the initial cell to a primitive cell of the lattice. The required transformation matrices are stored in the program.

3–5 The program transforms the primitive cell calculated in step 2 to a primitive cell that passes the main conditions for reduction specified in table 1.

6 The program transforms the cell to one that passes the special conditions for reduction specified in table 1. When this step has been completed, the computer program has reduced the input cell based on its geometry.

7 The results of the reduction procedure must be analyzed and interpreted taking into account the effects of the experimental errors. First, one must be certain that the geometrically reduced cell output by the computer program has been correctly normalized and the special conditions have been satisfied when the experimental errors are considered. In certain cases, further reduction may be indicated (this procedure is given in table 2). Finally, the metric lattice symmetry and other properties of the lattice may be deduced from the reduced cell.

Table 1. *Conditions for a reduced cell*

Cell s is specified by three noncoplanar vectors $\vec{a}, \vec{b}$, and $\vec{c}$ and cell matrix $S = (a \cdot a \; b \cdot b \; c \cdot c / b \cdot c \; a \cdot c \; a \cdot b)$ is defined by the dot products between these vectors.

To be reduced, the cell must be in normal representation (type I or II) and all the main and special conditions for the given cell type must be satisfied. The main conditions are used to establish that a cell is based on the three shortest lattice translations. The special conditions are used to select a unique cell when two or more cells in the lattice have the same numerical values for the cell edges. If inspection of the table indicates that a cell which is based on the three shortest vectors is not reduced, one can complete the reduction with the aid of the transformations given in table 2.

A. Positive reduced form, type I cell, all angles < 90 degrees

Main conditions:	$a \cdot a \leq b \cdot b \leq c \cdot c$;	$b \cdot c \leq 1/2\, b \cdot b$;	
	$a \cdot c \leq 1/2\, a \cdot a$;	$a \cdot b \leq 1/2\, a \cdot a$	
Special conditions:	(a) if $a \cdot a = b \cdot b$	then	$b \cdot c \leq a \cdot c$
	(b) if $b \cdot b = c \cdot c$	then	$a \cdot c \leq a \cdot b$
	(c) if $b \cdot c = 1/2\, b \cdot b$	then	$a \cdot b \leq 2\, a \cdot c$
	(d) if $a \cdot c = 1/2\, a \cdot a$	then	$a \cdot b \leq 2\, b \cdot c$
	(e) if $a \cdot b = 1/2\, a \cdot a$	then	$a \cdot c \leq 2\, b \cdot c$

B. Negative reduced form, type II cell, all angles ≥ 90 degrees

Main conditions:	(a) $a \cdot a \leq b \cdot b \leq c \cdot c$;	$b \cdot c \leq 1/2\, b \cdot b$;	
	$a \cdot c \leq 1/2\, a \cdot a$;	$a \cdot b \leq 1/2\, a \cdot a$	
	(b) $(\lvert b \cdot c \rvert + \lvert a \cdot c \rvert + \lvert a \cdot b \rvert) \leq 1/2(a \cdot a + b \cdot b)$		
Special conditions:	(a) if $a \cdot a = b \cdot b$	then	$\lvert b \cdot c \rvert \leq \lvert a \cdot c \rvert$
	(b) if $b \cdot b = c \cdot c$	then	$\lvert a \cdot c \rvert \leq \lvert a \cdot b \rvert$
	(c) if $\lvert b \cdot c \rvert = 1/2\, b \cdot b$	then	$a \cdot b = 0$
	(d) if $\lvert a \cdot c \rvert = 1/2\, a \cdot a$	then	$a \cdot b = 0$
	(e) if $\lvert a \cdot b \rvert = 1/2\, a \cdot a$	then	$a \cdot c = 0$
	(f) if $(\lvert b \cdot c \rvert + \lvert a \cdot c \rvert + \lvert a \cdot b \rvert) = 1/2(a \cdot a + b \cdot b)$	then	$a \cdot a \leq 2 \lvert a \cdot c \rvert + \lvert a \cdot b \rvert$

Table 2.[+] *Transformations for determining the reduced cell from an unreduced cell that is based on the shortest three translations of the lattice*

This table includes the transformation matrices that are required to convert a non-standard cell to a type I or a type II cell and the matrices that are required to satisfy the special conditions for reduction.

The cells **s** and **s′** are defined by three noncoplanar vectors $(\vec{a}, \vec{b}, \vec{c})$ and $(\vec{A}, \vec{B}, \vec{C})$, respectively. The cell matrices $\mathbf{S} = (a\cdot a \quad b\cdot b \quad c\cdot c / b\cdot c \quad a\cdot c \quad a\cdot b)$ and $\mathbf{S}' = (A\cdot A \quad B\cdot B \quad C\cdot C / B\cdot C \quad A\cdot C \quad A\cdot B)$ are defined by the dot products of the vectors defining the cells.

The relations between the scalars in column 4 are not intended to show the vector operations resulting from the application of a matrix in column 3 to cell **s**. Instead, column 4 gives the numerical values of $B\cdot C$, $A\cdot C$, $A\cdot B$ in terms of the numerical values of $b\cdot c$, $a\cdot c$, and $a\cdot b$. The values for $A\cdot A$, $B\cdot B$, and $C\cdot C$ are not given in column 4 since numerically $A\cdot A = a\cdot a$, $B\cdot B = b\cdot b$, and $C\cdot C = c\cdot c$. These equalities hold only for those cases in which the relations between the scalars given in column 2 are exact.

To use this table, calculate the cell matrix **S** and check the scalar relations in column 2. If a given relationship is true, the cell is not reduced and it must be transformed by the matrix given in column 3 to give cell **s′** having the cell type specified in column 5. The resultant cell matrix **S′** may be obtained from the data in column 4. The cell **s′** and cell matrix **S′** are relabeled as **s** and **S**, respectively. The process is repeated in an iterative manner until the cell is reduced. In practice, the following strategy is convenient: 1) set the dot products in **S** to ideal values (i.e., set the relations between the scalars for **S** to be exactly those given in the second column) considering the effects of experimental error; 2) use the table in an iterative manner (described above) until the reduction process is complete; 3) obtain the unidealized reduced cell by applying the final transformation matrix to the original unreduced cell.

Type of Cell **s**	Relations between Scalars in Matrix **S**	Transformation Matrix **s** to **s′**	Resultant Unsymmetrical Scalars in Matrix **S′**	Type of Cell **s′**
non-standard	$b\cdot c > 0,\ a\cdot c < 0,\ a\cdot b < 0$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$B\cdot C = b\cdot c$ $A\cdot C = \lvert a\cdot c\rvert$ $A\cdot B = \lvert a\cdot b\rvert$	I
non-standard	$b\cdot c < 0,\ a\cdot c > 0,\ a\cdot b < 0$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$B\cdot C = \lvert b\cdot c\rvert$ $A\cdot C = a\cdot c$ $A\cdot B = \lvert a\cdot b\rvert$	I
non-standard	$b\cdot c < 0,\ a\cdot c < 0,\ a\cdot b > 0$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$B\cdot C = \lvert b\cdot c\rvert$ $A\cdot C = \lvert a\cdot c\rvert$ $A\cdot B = a\cdot b$	I
non-standard	a) $b\cdot c \leq 0,\ a\cdot c > 0,\ a\cdot b > 0$ or b) $b\cdot c < 0,\ a\cdot c > 0,\ a\cdot b = 0$ or c) $b\cdot c < 0,\ a\cdot c = 0,\ a\cdot b > 0$ or d) $b\cdot c = 0,\ a\cdot c > 0,\ a\cdot b = 0$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$B\cdot C = b\cdot c$ $A\cdot C = -a\cdot c$ $A\cdot B = -a\cdot b$	II
non-standard	a) $b\cdot c > 0,\ a\cdot c \leq 0,\ a\cdot b > 0$ or b) $b\cdot c > 0,\ a\cdot c < 0,\ a\cdot b = 0$ or c) $b\cdot c = 0,\ a\cdot c < 0,\ a\cdot b > 0$ or d) $b\cdot c = 0,\ a\cdot c = 0,\ a\cdot b > 0$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$B\cdot C = -b\cdot c$ $A\cdot C = a\cdot c$ $A\cdot B = -a\cdot b$	II
non-standard	a) $b\cdot c > 0,\ a\cdot c > 0,\ a\cdot b \leq 0$ or b) $b\cdot c > 0,\ a\cdot c = 0,\ a\cdot b < 0$ or c) $b\cdot c = 0,\ a\cdot c > 0,\ a\cdot b < 0$ or d) $b\cdot c > 0,\ a\cdot c = 0,\ a\cdot b = 0$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$B\cdot C = -b\cdot c$ $A\cdot C = -a\cdot c$ $A\cdot B = a\cdot b$	II
I or II	$a\cdot a = b\cdot b$ and $\lvert a\cdot c\rvert < \lvert b\cdot c\rvert$	$\begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$B\cdot C = a\cdot c$ $A\cdot C = b\cdot c$ $A\cdot B = a\cdot b$	I or II, respectively
I or II	$b\cdot b = c\cdot c$ and $\lvert a\cdot b\rvert < \lvert a\cdot c\rvert$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}$	$B\cdot C = b\cdot c$ $A\cdot C = a\cdot b$ $A\cdot B = a\cdot c$	I or II, respectively

Table 2.[+] *Transformations for determining the reduced cell from an unreduced cell that is based on the shortest three translations of the lattice—Continued*

Type of Cell s	Relations between Scalars in Matrix S		Transformation Matrix s to s′	Resultant Unsymmetrical Scalars in Matrix S′	Type of Cell s′
I	$b\cdot c = b\cdot b/2$ $2a\cdot c < a\cdot b$	and	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & -1 & 1 \end{pmatrix}$	$B\cdot C = b\cdot b/2$ $A\cdot C = a\cdot b - a\cdot c$ $A\cdot B = a\cdot b$	I
I	$a\cdot c = a\cdot a/2$ $2b\cdot c < a\cdot b$	and	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ -1 & 0 & 1 \end{pmatrix}$	$B\cdot C = a\cdot b - b\cdot c$ $A\cdot C = a\cdot a/2$ $A\cdot B = a\cdot b$	I
I	$a\cdot b = a\cdot a/2$ $2b\cdot c < a\cdot c$	and	$\begin{pmatrix} -1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$B\cdot C = a\cdot c - b\cdot c$ $A\cdot C = a\cdot c$ $A\cdot B = a\cdot a/2$	I
II	$b\cdot c = -b\cdot b/2$ $a\cdot b \neq 0$	and	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & -1 & -1 \end{pmatrix}$	$B\cdot C = b\cdot b/2$ $A\cdot C = \lvert a\cdot c\rvert + \lvert a\cdot b\rvert$ $A\cdot B = \lvert a\cdot b\rvert$	I
II	$a\cdot c = -a\cdot a/2$ $a\cdot b \neq 0$	and	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 0 & -1 \end{pmatrix}$	$B\cdot C = \lvert b\cdot c\rvert + \lvert a\cdot b\rvert$ $A\cdot C = a\cdot a/2$ $A\cdot B = \lvert a\cdot b\rvert$	I
II	$a\cdot b = -a\cdot a/2$ $a\cdot c \neq 0$	and	$\begin{pmatrix} -1 & 0 & 0 \\ -1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$B\cdot C = \lvert b\cdot c\rvert + \lvert a\cdot c\rvert$ $A\cdot C = \lvert a\cdot c\rvert$ $A\cdot B = a\cdot a/2$	I
II	$a\cdot a + b\cdot b =$ $2(\lvert b\cdot c\rvert + \lvert a\cdot c\rvert + \lvert a\cdot b\rvert)$ $2\lvert a\cdot c\rvert + \lvert a\cdot b\rvert < a\cdot a$	and	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 1 & 1 & 1 \end{pmatrix}$	$B\cdot C = \lvert a\cdot b\rvert + \lvert b\cdot c\rvert - b\cdot b$ $A\cdot C = \lvert a\cdot b\rvert + \lvert a\cdot c\rvert - a\cdot a$ $A\cdot B = a\cdot b$	II

[+] Table 5.1.2.2 of the *International Tables for X-ray Crystallography* (1969 *a*) modified to include published revisions and additional information.

Table 3. *Metric classification of the 44 reduced forms*

This Table is reprinted from Mighell & Rodgers, 1980; based on Table 5.1.3.1 prepared by A. D. Mighell, A. Santoro and J. D. H. Donnay for the *International Tables for X-ray Crystallography* (1969 *a*) and published revisions.

Reduced Form No.	Reduced Form Matrix				Reduced Form Type	Bravais Lattice		Cell Transformation Reduced → Conventional
	First Row	Second Row						
	$\mathbf{a}\cdot\mathbf{a}$ $\mathbf{b}\cdot\mathbf{b}$ $\mathbf{c}\cdot\mathbf{c}$	$\mathbf{b}\cdot\mathbf{c}$	$\mathbf{a}\cdot\mathbf{c}$	$\mathbf{a}\cdot\mathbf{b}$				
$a=b=c$								
1	$a\cdot a$ $a\cdot a$ $a\cdot a$	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	+	Cubic	F	$1\bar{1}1/11\bar{1}/\bar{1}11$
2	$a\cdot a$ $a\cdot a$ $a\cdot a$	$b\cdot c$	$b\cdot c$	$b\cdot c$	+	Rhombohedral	hR	$1\bar{1}0/\bar{1}01/\bar{1}\bar{1}\bar{1}$
3	$a\cdot a$ $a\cdot a$ $a\cdot a$	0	0	0	-	Cubic	P	100/010/001
4	$a\cdot a$ $a\cdot a$ $a\cdot a$	$-\lvert b\cdot c\rvert$	$-\lvert b\cdot c\rvert$	$-\lvert b\cdot c\rvert$	-	Rhombohedral	hR	$1\bar{1}0/\bar{1}01/\bar{1}\bar{1}\bar{1}$
5	$a\cdot a$ $a\cdot a$ $a\cdot a$	$-\frac{a\cdot a}{3}$	$-\frac{a\cdot a}{3}$	$-\frac{a\cdot a}{3}$	-	Cubic	I	101/110/011
6	$a\cdot a$ $a\cdot a$ $a\cdot a$	$\frac{-a\cdot a+\lvert a\cdot b\rvert}{2}$	$\frac{-a\cdot a+\lvert a\cdot b\rvert}{2}$	$-\lvert a\cdot b\rvert$	-	Tetragonal	I	011/101/110
7	$a\cdot a$ $a\cdot a$ $a\cdot a$	$-\lvert b\cdot c\rvert$	$\frac{-a\cdot a+\lvert b\cdot c\rvert}{2}$	$\frac{-a\cdot a+\lvert b\cdot c\rvert}{2}$	-	Tetragonal	I	101/110/011
8	$a\cdot a$ $a\cdot a$ $a\cdot a$	$-\lvert b\cdot c\rvert$	$-\lvert a\cdot c\rvert$	$-(\lvert a\cdot a\rvert-\lvert b\cdot c\rvert-\lvert a\cdot c\rvert)$	-	Orthorhombic	I	$\bar{1}\bar{1}0/\bar{1}0\bar{1}/0\bar{1}\bar{1}$
$a=b$								
9	$a\cdot a$ $a\cdot a$ $c\cdot c$	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	+	Rhombohedral	hR	$100/\bar{1}10/\bar{1}\bar{1}3$
10	$a\cdot a$ $a\cdot a$ $c\cdot c$	$b\cdot c$	$b\cdot c$	$a\cdot b$	+	Monoclinic	C**	$110/1\bar{1}0/00\bar{1}$
11	$a\cdot a$ $a\cdot a$ $c\cdot c$	0	0	0	-	Tetragonal	P	100/010/001
12	$a\cdot a$ $a\cdot a$ $c\cdot c$	0	0	$-\frac{a\cdot a}{2}$	-	Hexagonal	P	100/010/001
13	$a\cdot a$ $a\cdot a$ $c\cdot c$	0	0	$-\lvert a\cdot b\rvert$	-	Orthorhombic	C	$110/\bar{1}10/001$
14	$a\cdot a$ $a\cdot a$ $c\cdot c$	$-\lvert b\cdot c\rvert$	$-\lvert b\cdot c\rvert$	$-\lvert a\cdot b\rvert$	-	Monoclinic	C**	$110/\bar{1}10/001$
15	$a\cdot a$ $a\cdot a$ $c\cdot c$	$-\frac{a\cdot a}{2}$	$-\frac{a\cdot a}{2}$	0	-	Tetragonal	I	100/010/112
16	$a\cdot a$ $a\cdot a$ $c\cdot c$	$-\lvert b\cdot c\rvert$	$-\lvert b\cdot c\rvert$	$-(a\cdot a-2\lvert b\cdot c\rvert)$	-	Orthorhombic	F	$\bar{1}\bar{1}0/1\bar{1}0/112$
17	$a\cdot a$ $a\cdot a$ $c\cdot c$	$-\lvert b\cdot c\rvert$	$-\lvert a\cdot c\rvert$	$-(a\cdot a-\lvert b\cdot c\rvert-\lvert a\cdot c\rvert)$	-	Monoclinic	I††	$\bar{1}0\bar{1}/\bar{1}\bar{1}0/011$
$b=c$								
18	$a\cdot a$ $b\cdot b$ $b\cdot b$	$\frac{a\cdot a}{4}$	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	+	Tetragonal	I	$0\bar{1}1/1\bar{1}\bar{1}/100$
19	$a\cdot a$ $b\cdot b$ $b\cdot b$	$b\cdot c$	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	+	Orthorhombic	I	$\bar{1}00/0\bar{1}1/\bar{1}11$
20	$a\cdot a$ $b\cdot b$ $b\cdot b$	$b\cdot c$	$a\cdot c$	$a\cdot c$	+	Monoclinic	C†	$011/01\bar{1}/\bar{1}00$
21	$a\cdot a$ $b\cdot b$ $b\cdot b$	0	0	0	-	Tetragonal	P	010/001/100
22	$a\cdot a$ $b\cdot b$ $b\cdot b$	$-\frac{b\cdot b}{2}$	0	0	-	Hexagonal	P	010/001/100
23	$a\cdot a$ $b\cdot b$ $b\cdot b$	$-\lvert b\cdot c\rvert$	0	0	-	Orthorhombic	C	$011/0\bar{1}1/100$
24	$a\cdot a$ $b\cdot b$ $b\cdot b$	$-\frac{b\cdot b-\frac{a\cdot a}{3}}{2}$	$-\frac{a\cdot a}{3}$	$-\frac{a\cdot a}{3}$	-	Rhombohedral	hR	$121/0\bar{1}1/100$
25	$a\cdot a$ $b\cdot b$ $b\cdot b$	$-\lvert b\cdot c\rvert$	$-\lvert a\cdot c\rvert$	$-\lvert a\cdot c\rvert$	-	Monoclinic	C†	$011/0\bar{1}1/100$

Table 3. *Metric classification of the 44 reduced forms*—Continued

Reduced Form No.	Reduced Form Matrix				Reduced Form Type	Bravais Lattice	Cell Transformation Reduced → Conventional
	First Row†††	Second Row					
	a·a b·b c·c	b·c	a·c	a·b			
a≤b≤c 26	a·a b·b c·c	$\frac{a\cdot a}{4}$	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	+	Orthorhombic F	100/$\bar{1}$20/$\bar{1}$02
27	a·a b·b c·c	b·c	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	+	Monoclinic I***	0$\bar{1}$1/$\bar{1}$00/1$\bar{1}\bar{1}$
28	a·a b·b c·c	$\frac{a\cdot b}{2}$	$\frac{a\cdot a}{2}$	a·b	+	Monoclinic C	$\bar{1}$00/$\bar{1}$02/010
29	a·a b·b c·c	$\frac{a\cdot c}{2}$	a·c	$\frac{a\cdot a}{2}$	+	Monoclinic C	100/1$\bar{2}$0/00$\bar{1}$
30	a·a b·b c·c	$\frac{b\cdot b}{2}$	$\frac{a\cdot b}{2}$	a·b	+	Monoclinic C	010/01$\bar{2}$/$\bar{1}$00
31	a·a b·b c·c	b·c	a·c	a·b	+	Triclinic P	100/010/001
32	a·a b·b c·c	0	0	0	-	Orthorhombic P	100/010/001
33	a·a b·b c·c	0	-|a·c|	0	-	Monoclinic P	100/010/001
34	a·a b·b c·c	0	0	-|a·b|	-	Monoclinic P	$\bar{1}$00/00$\bar{1}$/0$\bar{1}$0
35	a·a b·b c·c	-|b·c|	0	0	-	Monoclinic P	0$\bar{1}$0/$\bar{1}$00/00$\bar{1}$
36	a·a b·b c·c	0	$-\frac{a\cdot a}{2}$	0	-	Orthorhombic C	100/$\bar{1}$0$\bar{2}$/010
37	a·a b·b c·c	-|b·c|	$-\frac{a\cdot a}{2}$	0	-	Monoclinic C*	102/100/010
38	a·a b·b c·c	0	0	$-\frac{a\cdot a}{2}$	-	Orthorhombic C	$\bar{1}$00/120/00$\bar{1}$
39	a·a b·b c·c	-|b·c|	0	$-\frac{a\cdot a}{2}$	-	Monoclinic C**	$\bar{1}\bar{2}$0/$\bar{1}$00/00$\bar{1}$
40	a·a b·b c·c	$-\frac{b\cdot b}{2}$	0	0	-	Orthorhombic C	0$\bar{1}$0/012/$\bar{1}$00
41	a·a b·b c·c	$-\frac{b\cdot b}{2}$	-|a·c|	0	-	Monoclinic C†	0$\bar{1}\bar{2}$/0$\bar{1}$0/$\bar{1}$00
42	a·a b·b c·c	$-\frac{b\cdot b}{2}$	$-\frac{a\cdot a}{2}$	0	-	Orthorhombic I	$\bar{1}$00/0$\bar{1}$0/112
43	a·a b·b c·c	$-\frac{b\cdot b-\lvert a\cdot b\rvert}{2}$	$-\frac{a\cdot a-\lvert a\cdot b\rvert}{2}$	-|a·b|	-	Monoclinic I	$\bar{1}$00/$\bar{1}\bar{1}\bar{2}$/0$\bar{1}$0
44	a·a b·b c·c	-|b·c|	-|a·c|	-|a·b|	-	Triclinic P	100/010/001

† If $a\cdot a < 4|a\cdot c|$
* If $b\cdot b < 4|b\cdot c|$
** If $c\cdot c < 4|b\cdot c|$
} Premultiply Table Matrix by 00$\bar{1}$/010/101 (I centered)

†† If $3a\cdot a < c\cdot c + 2|a\cdot c|$
*** If $3b\cdot b < c\cdot c + 2|b\cdot c|$
} Premultiply Table Matrix by $\bar{1}$0$\bar{1}$/010/100 (C centered)

††† No required relationships between symmetrical scalars for reduced forms 26-44.

C. Derivative supercells and subcells

1. Theory and computer algorithm

If a three by three upper-triangular matrix Q with integer elements and a determinant of n (n = a positive integer greater than 1) is used to transform a primitive cell of the original lattice (PCOL), one obtains a derivative supercell of n times the volume of the PCOL. If the transpose of the inverse of Q is used to transform a PCOL, one obtains a derivative subcell of 1/n times the volume of the PCOL (Santoro & Mighell, 1972). It has been shown that unique sets of upper-triangular matrices can conveniently be generated for each value of the determinant (Santoro & Mighell, 1973). There are 7,13,35,31,91,57,155,130 unique upper-triangular matrices with determinants of 2,3,4,5,6,7,8,9, respectively. Each set of upper-triangular matrices can then be used to obtain all the unique supercells of n times the volume of the PCOL. By using the transpose of the inverse of each of these matrices, one can calculate all the unique subcells of 1/n times the volume of the PCOL. In the generation of the derivative cells, sets of these matrices can be used to transform any PCOL but they must be applied to the same cell. (The *NBS*LATTICE* program applies these matrices to the reduced, primitive cell of the original lattice.) Table 4 gives the upper-triangular matrices for determinants with n of 2,3 and 4. For a general triclinic lattice with no specialization in the reduced form, the derivative supercells and subcells for each value of the determinant are metrically different. However, for certain specialized triclinic lattices or for lattices of higher metric symmetry, some of the derivative cells are metrically identical although they are oriented differently in space.

A summary of the procedure used by the program to calculate derivative supercells and subcells is outlined in figure 2. The program first calculates the reduced cell of the original lattice, (RCOL) steps 1–6. Next, the specified set(s) of upper-triangular matrices are generated (step 7). By using the upper-triangular matrices, set(s) of supercells and/or subcells are generated and reduced (step 8). With a given upper-triangular matrix, one can determine a superlattice and a sublattice. In the program, each supercell is calculated in a two-step process: first, an intermediate supercell is calculated by transforming the RCOL by an upper-triangular matrix; second, the intermediate cell is reduced to yield a reduced supercell of the lattice. Each subcell is calculated in a similar manner using a three-step process: first, the transpose of the inverse of each upper-triangular matrix is calculated; second, an intermediate subcell is calculated by transforming the RCOL by the transpose of the inverse of the upper-triangular matrix; and third, the intermediate subcell is reduced. The present version of the program will calculate all the upper-triangular matrices with determinants ranging from 2 to 9. Thus, supercells with n (n = 2 to 9) times the volume of the RCOL and/or subcells with 1/n (n = 2 to 9) times the volume of the RCOL can be determined.

2. Uses of derivative supercells and subcells

There are many reasons for calculating derivative cells of the lattice. For example, as outlined below, the calculation of derivative cells can assist in obtaining the correct cell of the lattice and in the identification of unknown compounds. Additional discussions and examples are given in section II.

a. Derivative cells can lead to the determination of the correct cell of the lattice.

Cells determined from single-crystal and powder data are sometimes derivative cells of the lattice. However, it is still possible to deduce the correct cell by systematically calculating derivative cells. For example, a cell determined on a single-crystal diffractometer can be a subcell of the lattice; this occurs if one has determined a supercell in reciprocal space (i.e. by missing rows of diffraction intensities, etc.). If a subcell having 1/2 the volume of the correct cell has been determined, the correct cell can be found by calculating the 7 possible supercells of the experimentally determined subcell. One of the 7 generated supercells is the correct cell of the lattice. A cell determined by powder-indexing procedures can also be a derivative subcell, supercell, or composite cell of the lattice. By systematically calculating derivative cells from the initial powder cell, one can often deduce the correct cell.

b. Derivative cells can assist in the identification of unknown compounds by using the NBS Crystal Data File.

The ability to calculate derivative cells is important in the identification of compounds. One must be careful when identifying unknown materials by using the *NBS Crystal Data File* because the unknown cell or the corresponding entry in the File may be in a derivative relationship (i.e., one may be the derivative lattice of the other). Therefore, one may wish to match routinely the reduced cell and selected derivative cells of the unknown against the File.

Figure 2. *Derivative supercells and subcells*

Notes:

1–6 Same steps as in the reduction procedure outlined in figure 1.

7 The required upper-triangular matrices generated by the computer program are stored in arrays. The program will not calculate upper-triangular matrices with determinants less than 2 or exceeding 9.

8 The specified derivative supercells and/or subcells are calculated by transforming the reduced cell of the original lattice (RCOL) by the appropriate matrices. For each supercell, an upper-triangular matrix is used; for each subcell, the transpose of the inverse of the upper-triangular matrix is used. Each derivative cell is then transformed to the reduced cell of the derivative lattice.

As indicated by the notations, the program can carry out calculations in either the supercell (8a...8h), the subcell (8a'...8h'), or the supercell and subcell (8a...8h,8a'...8h') series. One can calculate derivative lattices starting at any point and ending at any point within a given series. For example, one can carry out step 8a only, or all the steps 8a...8h, or two or more adjacent steps, such as 8b, 8c and 8d.

Figure 2. *Derivative supercells and subcells*—Continued

8a 7 supercells of two times the volume of the RCOL (step 6) are calculated and reduced in a two-step process: first, the 7 unique upper-triangular matrices (step 7) with a determinant of 2 are used to transform the RCOL to 7 derivative supercells; second, the 7 derivative supercells are then reduced.

8a′ 7 subcells of 1/2 the volume of the RCOL (step 6) are calculated and reduced in a three-step process: first, the transpose of the inverse of each of the 7 unique upper-triangular matrices (step 7) is calculated; second, the transposes of the inverses of these matrices are then used to transform the RCOL to 7 derivative subcells with 1/2 the volume of the RCOL; third, the 7 derivative subcells are then reduced.

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.

8h 130 supercells of 9 times the volume of the RCOL (step 6) are calculated and reduced in a two-step process as outlined in 8a except that 130 upper-triangular matrices are used.

8h′ 130 subcells of 1/9 the volume of the RCOL (step 6) are calculated and reduced in a three-step process as outlined in 8a′ except that 130 upper-triangular matrices are used.

9 The results must be analyzed and interpreted taking into account the effects of the experimental errors.

Table 4. *Unique* **Q** *matrices generating superlattices for* $|\mathbf{Q}| = 2, 3, 4$

For each value of **Q**, the matrices can be applied to any primitive cell of the original lattice, but they must be applied to the same cell.

$\lvert\mathbf{Q}\rvert = 2$	$\lvert\mathbf{Q}\rvert = 4$	$\lvert\mathbf{Q}\rvert = 4$ (cont.)
(100 / 010 / 002)	(100 / 010 / 004)	(111 / 021 / 002)
(100 / 011 / 002)	(100 / 011 / 004)	(100 / 040 / 001)
(101 / 010 / 002)	(100 / 012 / 004)	(110 / 040 / 001)
(101 / 011 / 002)	(100 / 013 / 004)	(120 / 040 / 001)
(100 / 020 / 001)	(101 / 010 / 004)	(130 / 040 / 001)
(110 / 020 / 001)	(101 / 011 / 004)	(200 / 010 / 002)
(200 / 010 / 001)	(101 / 012 / 004)	(200 / 011 / 002)
	(101 / 013 / 004)	(201 / 010 / 002)
$\lvert\mathbf{Q}\rvert = 3$	(102 / 010 / 004)	(201 / 011 / 002)
	(102 / 011 / 004)	(200 / 020 / 001)
(100 / 010 / 003)	(102 / 012 / 004)	(210 / 020 / 001)
(100 / 011 / 003)	(102 / 013 / 004)	(400 / 010 / 001)
(100 / 012 / 003)	(103 / 010 / 004)	
(101 / 010 / 003)	(103 / 011 / 004)	
(101 / 011 / 003)	(103 / 012 / 004)	
(101 / 012 / 003)	(103 / 013 / 004)	
(102 / 010 / 003)	(100 / 020 / 002)	
(102 / 011 / 003)	(100 / 021 / 002)	
(102 / 012 / 003)	(101 / 020 / 002)	
(100 / 030 / 001)	(101 / 021 / 002)	
(110 / 030 / 001)	(110 / 020 / 002)	
(120 / 030 / 001)	(110 / 021 / 002)	
(300 / 010 / 001)	(111 / 020 / 002)	

D. Operation of the Program

1. General

There are two types of input lines required to execute the reduction and derivative supercell and subcell (RSS) program function. The first input line is a Program Control Line that specifies the type of program function and the number of problems to be solved. The second type of input line is an RSS Control Line that defines the input lattice and the calculations to be performed (i.e., various combinations of reduction, supercell, subcell calculations). For N problems specified on the Program Control Line, N RSS Control Lines must follow ($1 \leq N \leq 20$). Within a single computer run, the RSS program function may be executed any number of times. A description of the formats for the input lines and typical examples are given below.

2. Description of input lines

a. Program Control Line

The Program Control Line specifies the type of program function and the number of problems to be solved. For each execution of the RSS program function within a single computer run, only one Program Control Line is required.

Program Control Line
Format(A5,3X,I2)

	Column	Format	Item
1	1–5	A5	Type of program function 'LM ' = Lattice Matching 'RSS ' = Reduction and Derivative Supercell and Subcell 'TRANS' = Cell Transformation 'INV ' = Matrix Inversion
	6–8	3X	Blank
2	9–10	I2	Number of problems

Notes:

1 The RSS program function is specified by 'RSS ' in columns 1–5.

2 The number of problems specified in a single execution of the RSS program function may range between 1 and 20.

b. RSS Control Line

The RSS Control Line defines the input lattice and the derivative lattices to be calculated. The lattice is defined by specifying the cell centering and all six unit cell parameters. The program will always carry out the cell reduction calculations. To calculate derivative lattices, it is necessary to tell the program whether to calculate supercells, subcells, or both supercells and subcells. In addition, for derivative lattice calculations, it is necessary to tell the program which multiples of the reduced cell volume (V) should be considered. Supercells having 2 to 9 times the volume of the reduced input cell and/or subcells having 1/2 to 1/9 times the volume of the reduced input cell may be calculated. There are 7 unique derivative lattices (supercells or subcells, respectively) having 2 or 1/2 times the volume of the reduced input cell, 13 derivative lattices with 3V or 1/3V, 35 with 4V or 1/4V, 31 with 5V or 1/5V, 91 with 6V or 1/6V, 57 with 7V or 1/7V, 155 with 8V or 1/8V, and 130 with 9V or 1/9V. For N problems specified on the Program Control Line, N RSS Control Lines must follow ($1 \leq N \leq 20$).

RSS Control Line
Format(I1,2X,2I1,3X,2A1,6F10.2)

	Column	Format	Item
1	1	I1	Blank/1/2/3/ Blank = Reduction 1 = Reduction+supercells 2 = Reduction+subcells 3 = Reduction+supercells, subcells
	2–3	2X	Blank
2	4	I1	Blank/2/3/4/5/6/7/8/9/ Initial value (n1) to define the range of volumes for calculated derivative lattices.
3	5	I1	Blank/2/3/4/5/6/7/8/9/ Final value (n2) to define the range of volumes for calculated derivative lattices.
	6–8	3X	Blank
4	9	A1	P/A/B/C/F/I/R/ Cell centering
5	10	A1	R/H/ Rhombohedral/Hexagonal/ metric axes. Used only for rhombohedral lattices.
6	11–20	F10.2	a (Å)
7	21–30	F10.2	b
8	31–40	F10.2	c
9	41–50	F10.2	alpha (°)
10	51–60	F10.2	beta
11	61–70	F10.2	gamma

Notes:

1 If only a reduction is to be carried out, this field is left blank. If derivative lattices are to be calculated, then a 1, 2 or 3 is used for supercells, or subcells, or both supercells and subcells, respectively.

2 If only a reduction is to be carried out, this field is left blank. If derivative lattices are to be calculated, use an integer (n1) from 2 to 9.

3 If only a reduction is to be carried out, this field is left blank. If derivative lattices are to be calculated, use an integer (n2) from 2 to 9, but greater than or equal to n1.

Notes (cont.)

2–3 These two integers (n1 and n2) are used to define the range of volumes for the derivative lattices to be calculated. The supercells to be calculated will have volumes ranging from (n1)V to (n2)V while the volumes for the subcells to be calculated will range from (1/n1)V to (1/n2)V.

4 To define the lattice, both the cell and cell centering are required. A symbol specifying the cell centering must be placed in columns 9 and 10. A one character symbol is used for P,A,B,C,F, and I centered cells. For a cell defining a rhombohedral lattice, a two character symbol is required (RR or RH); the first character of this symbol ('R') is placed in column 9.

5 Column 10 is left blank unless the input cell defines a rhombohedral lattice. For a cell defining a rhombohedral lattice, an 'R' is placed in column 10 if the lattice is defined by a primitive rhombohedral cell (rhombohedral axes), or an 'H' is used if the lattice is defined by a triply primitive rhombohedral cell (metrically hexagonal axes).

6–8 Cell edges (Å).

9–11 Cell angles (°). Decimal numbers must be used for fractions of a degree. All six cell parameters must always be specified regardless of the crystal symmetry.

3. Example of input flowstream

```
.........1.........1.........1.........1.........1.........1.........1

1   RSS       1
2             P 4.99       9.36       9.19       102.1      91.5       68.0
3   RSS       3
4             A 15.380     14.225     9.309      90.00      94.20      90.00
5             RR16.11      16.11      16.11      115.10     115.10     115.10
6   3  23     RH9.139      9.139      15.536     90.00      90.00      120.00
```

Notes:

1 The 'RSS ' in columns 1–5 indicates that the RSS program function will be executed; the '1' in column 10 specifies that one RSS Control Line will follow (one problem is to be considered). At most 20 problems may be specified in a single execution of the RSS program function.

2 Since column 1 is blank, the cell will be reduced and no derivative lattices will be calculated. Columns 4–5 are also left blank for reduction-only calculations. The 'P ' in columns 9–10 indicates that the input cell is primitive. All six unit cell parameters are specified in columns 11–70.

3 The RSS program function will be executed a second time; in this case, three RSS Control Lines will follow (three independent problems are to be considered).

Notes (cont.)

4 This RSS Control Line directs the program to reduce an A-centered cell. Note that all six cell parameters are given even though this cell is metrically monoclinic. Even in the cubic crystal system, all six cell parameters must be given. Unit cell parameters are specified in columns 11–70.

5 The reduction of a rhombohedral cell will be carried out. A two character symbol 'RR' in columns 9–10 specifies that a primitive rhombohedral cell is used to define a rhombohedral lattice. All six unit cell parameters are given in columns 11–70.

6 The '3' in column 1 specifies that both supercells and subcells of the lattice will be calculated. The '23' in columns 4–5 signify that the 7 upper-triangular matrices with determinants of 2, and the 13 upper-triangular matrices with a determinant of 3 will be calculated. These matrices will be used in the calculation of the 7 derivative supercells of 2 times the volume of the reduced cell of the lattice and in the calculation of the 13 derivative supercells of 3 times the volume of the reduced cell of the lattice. The transpose of the inverse of the appropriate upper-triangular matrix will be used to calculate each of the 7 subcells of 1/2 times and the 13 subcells of 1/3 times the volume of the reduced cell of the lattice. Since the input lattice is rhombohedral, some of the derivative lattices will be metrically identical even though they are oriented differently in space. A two character symbol 'RH' in columns 9–10 specifies that a triply primitive rhombohedral cell (metrically hexagonal axes) is used to define a rhombohedral lattice. All six unit cell parameters are given in columns 11–70.

4. Example of computer output

The computer output following this section results from the input flowstream discussed above (sec. III.D.3.).

a. Page 1 of computer output

A description of the output parameters is printed for the first execution of the RSS program function within a computer run.

b. Page 2 of computer output

One problem is to be considered during the first execution of the RSS program function. This problem is the reduction of a primitive, triclinic unit cell (CELL 1). In the computer output, V1 is the volume for the initial cell and V2 is the volume for the reduced cell (CELL 2). The matrix T1 is the identity matrix since a primitive unit cell was input. The transformation matrix T2 = (1 0 0 / -1 1 0 / 0 0 1) from the initial to the reduced cell has all integers and a determinant of +1. The reduced cell is of the type II with all angles greater than 90 degrees. The reduced cell matrix exhibits no specialization and corresponds to reduced form number 44 in table 3. The lattice is metrically triclinic; therefore, the crystal symmetry must be triclinic.

c. Page 3 of computer output

Three independent problems are to be considered in the second execution of the RSS program function. The first problem is the reduction of an A-centered monoclinic unit cell. The matrix T1 = (0 .5 -.5 / 0 .5 .5 / 1 0 0) transforms the initial A-centered cell (CELL 1) to a primitive cell of the lattice by removing the cell centering. The matrix T2 = (0 .5 -.5 / 0 -.5 -.5 / -1 0 0) transforms the initial A-centered cell to the reduced cell (CELL 2). In the computer output, V1 is the volume of the A-centered cell and V2 is the volume of the reduced cell. The reduced cell matrix corresponds to reduced form number 14 in table 3. Thus, the matrix (1 1 0 / -1 1 0 / 0 0 1) from table 3 will transform the reduced cell to a conventional C-centered monoclinic cell.

d. Page 4 of computer output

The reduction of a rhombohedral cell is the second of three independent problems to be considered in this execution of the RSS program function. The transformation matrix T2 = (1 1 1 / -1 0 0 / 0 -1 0) from the initial to the reduced cell has all integers and a determinant of +1 since a primitive, rhombohedral cell was used to define the rhombohedral lattice. The reduced cell matrix corresponds to reduced form number 24 in table 3. Note that, in this case, the reduced cell, based on the three shortest lattice translations, is not the primitive rhombohedral cell, but one with the a-cell parameter different from b and c, and alpha different from beta and gamma. The matrix (1 2 1 / 0 -1 1 / 1 0 0) obtained from table 3 may be used to transform the reduced cell to a triply primitive rhombohedral cell based on metrically hexagonal axes.

e. Pages 5–12 of computer output

The last independent problem to be considered illustrates the computer output for a derivative lattice calculation. In this case, both superlattices and sublattices are to be calculated. First, the initial cell is reduced. The matrix T1 transforms the input cell to a primitive cell of the lattice, while the matrix T2 transforms the input cell to the reduced cell of the lattice. Since a triply primitive cell (metrically hexagonal axes) was used to define the rhombohedral lattice (RH-centered), the reduced cell volume, V2, is one-third the volume for the input cell, V1. The reduced cell matrix corresponds to reduced form number 2 in table 3. In this case, the reduced cell is one with a = b = c and alpha = beta = gamma.

The output illustrates that, first, the initial cell (CELL 1) is transformed to the reduced cell of the original lattice (CELL 2, or more conveniently, 'RCOL'). The RCOL then becomes CELL 1 for the calculation of the derivative lattices.

The derivative supercells are calculated by transforming the RCOL by the unique upper-triangular matrices. First, the 7 supercells with volumes of 2 times the RCOL are determined; then the 13 supercells with volumes of 3 times the RCOL are calculated. After each supercell is calculated, it is then reduced. The reduced cell and reduced form corresponding to each superlattice are shown in the output. Two transformation matrices, T1 and T2, are given in the output along with the supercells. The matrix T1 is a unique upper-triangular matrix that transforms the RCOL to a derivative supercell which is not reduced; the matrix T2 transforms the RCOL to a reduced derivative supercell. Note that Supercell 9 corresponds to the triply primitive rhombohedral cell originally used to define the lattice (i.e., the input cell).

The computer output for the derivative subcells follows that for the supercells. First, the 7 subcells with volumes of 1/2 times the RCOL are determined; then the 13 subcells with volumes of 1/3 times the RCOL are calculated. After each subcell is calculated, it is then reduced. The reduced cell and reduced form corresponding to each sublattice are shown in the output. The matrix T1 is the transpose of the inverse of a unique upper-triangular matrix; T1 transforms the RCOL to a derivative subcell which is not reduced. The matrix T2 transforms the RCOL to a reduced derivative subcell.

Many of the derivative lattices are metrically identical even though they are oriented differently in space. This occurs for certain specialized lattices and for lattices with higher metric symmetry.

Section III.D.4.
Page 1

*** NBS*LATTICE ***

A PROGRAM TO ANALYZE LATTICE RELATIONSHIPS
Version of Spring, 1985

NBS Crystal Data Center
National Bureau of Standards
Reactor Radiation Division
Gaithersburg, MD 20899

** REDUCTION AND DERIVATIVE LATTICE **

These calculations fall into two categories:

I. Reduction of an input cell.

CELL 1 = Input cell. This cell may be primitive or centered (A,B,C,I,F,RR,RH).
CELL 2 = Reduced primitive cell of the lattice.
T 1 = A matrix that transforms CELL 1 to a primitive cell of the lattice.
T 2 = A matrix that transforms CELL 1 to CELL 2.

II. Calculation and reduction of a series of derivative supercells and/or subcells. These derivative cells are calculated from the reduced cell of the lattice (i.e. to carry out the Type II calculation, the program first carries out the Type I calculation).

CELL 1 = Reduced primitive cell (i.e. CELL 2 from Part I).
CELL 2 = Reduced supercell or subcell.
T 1 = A matrix that transforms CELL 1 to a supercell or subcell of the lattice.
T 2 = A matrix that transforms CELL 1 to CELL 2.

For CELL 1 and CELL 2, the output parameters given are: a, b, c, alpha, beta, gamma and volume. Cell edges are in angstroms and angles in degrees.

The reduced cell matrix is of the form:

a.a	b.b	c.c
b.c	a.c	a.b

Page 2

REDUCTION AND DERIVATIVE LATTICE

Number of independent problems to study = 1

1. REDUCTION

** Initial Cell is Primitive **

T 1=	1.00	.00	.00/	.00	1.00	.00/	.00	.00	1.00
T 2=	1.00	.00	.00/	-1.00	1.00	.00/	.00	.00	1.00
T 2 INV=	1.00	.00	.00/	1.00	1.00	.00/	.00	.00	1.00

** Cell Matrix **

CELL 1=	4.9900	9.3600	9.1900	102.00	91.500	68.000	V1=	388.49	24.900	77.517	84.456
CELL 2=	4.9900	8.8044	9.1900	102.06	91.500	99.702	V2=	388.49	-16.831	-1.200	-7.404

REOUCTION ANO OERIVATIVE LATTICE

Number of independent problems to study = 3

1. REOUCTION

** Initial Cell is A-Centered **

T 1=	.00	.50	-.50/	.00	.50	.50/	1.00	.00	.00
T 2=	.00	.50	-.50/	.00	-.50	-.50/	-1.00	.00	.00
T 2 INV=	.00	.00	-1.00/	1.00	-1.00	.00/	-1.00	-1.00	.00

** Cell Matrix **

CELL 1=	15.3800	14.2250	9.3090	90.000	94.200	90.000	V1=	2031.16	72.252	72.252	236.544
CELL 2=	8.5001	8.5001	15.3800	92.298	92.298	113.598	V2=	1015.58	-5.243	-5.243	-28.923

2. REOUCTION

** Initial Cell is Primitive **

T 1=	1.00	.00	.00/	.00	1.00	.00/	.00	.00	1.00
T 2=	1.00	1.00	1.00/	-1.00	.00	.00/	.00	-1.00	.00
T 2 INV=	.00	-1.00	.00/	.00	.00	-1.00/	1.00	1.00	1.00

** Cell Matrix **

CELL 1=	16.1100	16.1100	16.1100	115.100	115.100	115.100	V1=	2318.51	118.036	259.532	259.532
CELL 2=	10.8644	16.1100	16.1100	115.100	102.991	102.991	V2=	2318.51	-110.093	-39.345	-39.345

3. SUPERLATTICES for a given delta followed by SUBLATTICES for 1/delta

** Initial Cell is RH-Centered **

T 1=	.33	-.33	-.33/	-.67	-.33	-.33/	.33	.67	-.33
T 2=	.33	-.33	-.33/	-.67	-.33	-.33/	.33	.67	-.33
T 2 INV=	1.00	-1.00	.00/	-1.00	.00	1.00/	-1.00	-1.00	-1.00

** Cell Matrix **

CELL 1=	9.1390	9.1390	15.5360	90.000	90.000	120.000	V1=	1123.74	54.659	54.659	54.659
CELL 2=	7.3932	7.3932	7.3932	76.351	76.351	76.351	V2=	374.58	12.898	12.898	12.898

Superlattices for Delta = 2

***** Supercell 1 *****

T 1=	1.00	.00	.00/	.00	1.00	.00/	.00	.00	2.00
T 2=	1.00	.00	.00/	.00	1.00	.00/	.00	.00	2.00
T 2 INV=	1.00	.00	.00/	.00	1.00	.00/	.00	.00	.50

** Cell Matrix **

CELL 1=	7.3932	7.3932	7.3932	76.351	76.351	76.351	V1=	374.58	54.659	54.659	218.636
CELL 2=	7.3932	7.3932	14.7863	76.351	76.351	76.351	V2=	749.16	25.797	25.797	12.898

***** Supercell 2 *****

T 1=	1.00	.00	.00/	.00	1.00	1.00/	.00	.00	2.00
T 2=	1.00	.00	.00/	.00	-1.00	1.00/	.00	-1.00	-1.00
T 2 INV=	1.00	.00	.00/	.00	-.50	-.50/	.00	.50	-.50

** Cell Matrix **

CELL 1=	7.3932	7.3932	7.3932	76.351	76.351	76.351	V1=	374.58	54.659	83.521	135.115
CELL 2=	7.3932	9.1390	11.6239	90.000	107.468	90.000	V2=	749.16	.000	-25.797	.000

***** Supercell 3 *****

T 1=	1.00	.00	1.00/	.00	1.00	.00/	.00	.00	2.00
T 2=	.00	1.00	.00/	1.00	.00	-1.00/	-1.00	.00	-1.00
T 2 INV=	.00	.50	-.50/	1.00	.00	.00/	.00	-.50	-.50

** Cell Matrix **

CELL 1=	7.3932	7.3932	7.3932	76.351	76.351	76.351	V1=	374.58	54.659	83.521	135.115
CELL 2=	7.3932	9.1390	11.6239	90.000	107.468	90.000	V2=	749.16	.000	-25.797	.000

***** Supercell 4 *****

T 1=	1.00	.00	1.00/	.00	1.00	1.00/	.00	.00	2.00
T 2=	-1.00	1.00	.00/	.00	1.00	-1.00/	-1.00	.00	-1.00
T 2 INV=	-.50	.50	-.50/	.50	.50	-.50/	.50	-.50	-.50

** Cell Matrix **

```
CELL  1=    7.3932    7.3932    7.3932     76.351    76.351    76.351          V1=    374.58      83.521    83.521   135.115
CELL  2=    9.1390    9.1390   11.6239     66.852    66.852    60.000          V2=    749.16      41.761    41.761    41.761
```

***** Supercell 5 *****

```
T 1=       1.00    .00    .00/    .00   2.00    .00/    .00    .00   1.00
T 2=      -1.00    .00    .00/    .00    .00  -1.00/    .00  -2.00    .00
T 2 INV=  -1.00    .00    .00/    .00    .00   -.50/    .00  -1.00    .00
```

** Cell Matrix **

```
CELL  1=    7.3932    7.3932    7.3932     76.351    76.351    76.351          V1=    374.58      54.659    54.659   218.636
CELL  2=    7.3932    7.3932   14.7863     76.351    76.351    76.351          V2=    749.16      25.797    25.797    12.898
```

***** Supercell 6 *****

```
T 1=       1.00   1.00    .00/    .00   2.00    .00/    .00    .00   1.00
T 2=        .00    .00  -1.00/  -1.00   1.00    .00/   1.00   1.00    .00
T 2 INV=    .00   -.50    .50/    .00    .50    .50/  -1.00    .00    .00
```

** Cell Matrix **

```
CELL  1=    7.3932    7.3932    7.3932     76.351    76.351    76.351          V1=    374.58      54.659    83.521   135.115
CELL  2=    7.3932    9.1390   11.6239     90.000   107.468    90.000          V2=    749.16        .000   -25.797      .000
```

***** Supercell 7 *****

```
T 1=       2.00    .00    .00/    .00   1.00    .00/    .00    .00   1.00
T 2=        .00   1.00    .00/    .00    .00   1.00/   2.00    .00    .00
T 2 INV=    .00    .00    .50/   1.00    .00    .00/    .00   1.00    .00
```

** Cell Matrix **

```
CELL  1=    7.3932    7.3932    7.3932     76.351    76.351    76.351          V1=    374.58      54.659    54.659   218.636
CELL  2=    7.3932    7.3932   14.7863     76.351    76.351    76.351          V2=    749.16      25.797    25.797    12.898
```

Superlattices for Delta = 3

***** Supercell 1 *****

```
T 1=       1.00    .00    .00/    .00   1.00    .00/    .00    .00   3.00
T 2=       1.00    .00    .00/    .00  -1.00    .00/    .00   1.00  -3.00
T 2 INV=   1.00    .00    .00/    .00  -1.00    .00/    .00   -.33   -.33
```

** Cell Matrix **

```
CELL  1=    7.3932    7.3932    7.3932     76.351    76.351    76.351          V1=    374.58      54.659    54.659   469.200
CELL  2=    7.3932    7.3932   21.6610     95.721    99.270   103.649          V2=   1123.74     -15.964   -25.797   -12.898
```

***** Supercell 2 *****

```
T 1=       1.00    .00    .00/    .00   1.00   1.00/    .00    .00   3.00
T 2=       1.00    .00    .00/    .00   1.00   1.00/    .00  -1.00   2.00
T 2 INV=   1.00    .00    .00/    .00    .67   -.33/    .00    .33    .33
```

** Cell Matrix **

```
CELL  1=    7.3932    7.3932    7.3932     76.351    76.351    76.351          V1=    374.58      54.659   135.115   221.702
CELL  2=    7.3932   11.6239   14.8896     67.025    83.271    72.532          V2=   1123.74      67.557    12.898    25.797
```

***** Supercell 3 *****

```
T 1=      1.00    .00    .00/    .00   1.00   2.00/    .00    .00   3.00
T 2=      1.00    .00    .00/    .00   1.00  -1.00/  -1.00   1.00   2.00
T 2 INV=  1.00    .00    .00/    .33    .67    .33/    .33   -.33    .33

CELL  1=   7.3932    7.3932    7.3932     76.351    76.351    76.351
CELL  2=   7.3932    9.1390   17.3827    105.241    97.136    90.000
```

** Cell Matrix **

```
V1=   374.58     54.659    83.521   302.157
V2=  1123.74    -41.761   -15.964      .000
```

***** Supercell 4 *****

```
T 1=      1.00    .00   1.00/    .00   1.00    .00/    .00    .00   3.00
T 2=       .00  -1.00    .00/  -1.00    .00  -1.00/   1.00    .00  -2.00
T 2 INV=   .00   -.67    .33/  -1.00    .00    .00/    .00   -.33   -.33

CELL  1=   7.3932    7.3932    7.3932     76.351    76.351    76.351
CELL  2=   7.3932   11.6239   14.8896     67.025    83.271    72.532
```

** Cell Matrix **

```
V1=   374.58     54.659   135.115   221.702
V2=  1123.74     67.557    12.898    25.797
```

***** Supercell 5 *****

```
T 1=      1.00    .00   1.00/    .00   1.00   1.00/    .00    .00   3.00
T 2=      1.00  -1.00    .00/  -1.00    .00  -1.00/   1.00   1.00  -1.00
T 2 INV=   .33   -.33    .33/   -.67   -.33    .33/   -.33   -.67   -.33

CELL  1=   7.3932    7.3932    7.3932     76.351    76.351    76.351
CELL  2=   9.1390   11.6239   11.7550    100.882    90.000   113.148
```

** Cell Matrix **

```
V1=   374.58     83.521   135.115   138.180
V2=  1123.74    -25.797      .000   -41.761
```

***** Supercell 6 *****

```
T 1=      1.00    .00   1.00/    .00   1.00   2.00/    .00    .00   3.00
T 2=       .00   1.00  -1.00/   1.00    .00   1.00/   1.00  -1.00  -1.00
T 2 INV=   .33    .67    .33/    .67    .33   -.33/   -.33    .33   -.33

CELL  1=   7.3932    7.3932    7.3932     76.351    76.351    76.351
CELL  2=   9.1390   11.6239   11.7550    100.882    90.000   113.148
```

** Cell Matrix **

```
V1=   374.58     83.521   135.115   138.180
V2=  1123.74    -25.797      .000   -41.761
```

***** Supercell 7 *****

```
T 1=      1.00    .00   2.00/    .00   1.00    .00/    .00    .00   3.00
T 2=       .00  -1.00    .00/  -1.00    .00   1.00/  -1.00   1.00  -2.00
T 2 INV=  -.33   -.67   -.33/  -1.00    .00    .00/   -.33    .33   -.33

CELL  1=   7.3932    7.3932    7.3932     76.351    76.351    76.351
CELL  2=   7.3932    9.1390   17.3827    105.241    97.136    90.000
```

** Cell Matrix **

```
V1=   374.58     54.659    83.521   302.157
V2=  1123.74    -41.761   -15.964      .000
```

***** Supercell 8 *****

```
T 1=      1.00    .00   2.00/    .00   1.00   1.00/    .00    .00   3.00
T 2=     -1.00    .00   1.00/    .00  -1.00  -1.00/   1.00  -1.00   1.00
T 2 INV=  -.67   -.33    .33/   -.33   -.67   -.33/    .33   -.33    .33

CELL  1=   7.3932    7.3932    7.3932     76.351    76.351    76.351
```

** Cell Matrix **

```
V1=   374.58     83.521   135.115   138.180
```

```
CELL  2=    9.1390   11.6239   11.7550   100.882   90.000   113.148          V2=   1123.74      -25.797      .000    -41.761
```

```
                                  ***** Supercell   9 *****

T 1=        1.00    .00   2.00/    .00   1.00   2.00/    .00    .00   3.00
T 2=       -1.00    .00   1.00/    .00   1.00  -1.00/  -1.00  -1.00  -1.00
T 2 INV=   -.67   -.33   -.33/    .33    .67   -.33/    .33   -.33   -.33                    ** Cell Matrix **

CELL  1=    7.3932    7.3932    7.3932    76.351    76.351    76.351          V1=    374.58       83.521     83.521    241.367
CELL  2=    9.1390    9.1390   15.5360    90.000    90.000   120.000          V2=   1123.74         .000       .000    -41.761
```

```
                                  ***** Supercell  10 *****

T 1=        1.00    .00    .00/    .00   3.00    .00/    .00    .00   1.00
T 2=       -1.00    .00    .00/    .00    .00   1.00/    .00   3.00  -1.00
T 2 INV=   -1.00    .00    .00/    .00    .33    .33/    .00   1.00    .00                    ** Cell Matrix **

CELL  1=    7.3932    7.3932    7.3932    76.351    76.351    76.351          V1=    374.58       54.659     54.659    469.200
CELL  2=    7.3932    7.3932   21.6610    95.721    99.270   103.649          V2=   1123.74      -15.964    -25.797    -12.898
```

```
                                  ***** Supercell  11 *****

T 1=        1.00   1.00    .00/    .00   3.00    .00/    .00    .00   1.00
T 2=         .00    .00   1.00/   1.00   1.00    .00/  -1.00   2.00    .00
T 2 INV=     .00    .67   -.33/    .00    .33    .33/   1.00    .00    .00                    ** Cell Matrix **

CELL  1=    7.3932    7.3932    7.3932    76.351    76.351    76.351          V1=    374.58       54.659    135.115    221.702
CELL  2=    7.3932   11.6239   14.8896    67.025    83.271    72.532          V2=   1123.74       67.557     12.898     25.797
```

```
                                  ***** Supercell  12 *****

T 1=        1.00   2.00    .00/    .00   3.00    .00/    .00    .00   1.00
T 2=         .00    .00  -1.00/   1.00  -1.00    .00/  -2.00  -1.00   1.00
T 2 INV=    -.33    .33   -.33/   -.33   -.67   -.33/  -1.00    .00    .00                    ** Cell Matrix **

CELL  1=    7.3932    7.3932    7.3932    76.351    76.351    76.351          V1=    374.58       54.659     83.521    302.157
CELL  2=    7.3932    9.1390   17.3827   105.241    97.136    90.000          V2=   1123.74      -41.761    -15.964       .000
```

```
                                  ***** Supercell  13 *****

T 1=        3.00    .00    .00/    .00   1.00    .00/    .00    .00   1.00
T 2=         .00   1.00    .00/    .00    .00  -1.00/  -3.00    .00   1.00
T 2 INV=     .00   -.33   -.33/   1.00    .00    .00/    .00  -1.00    .00                    ** Cell Matrix **

CELL  1=    7.3932    7.3932    7.3932    76.351    76.351    76.351          V1=    374.58       54.659     54.659    469.200
CELL  2=    7.3932    7.3932   21.6610    95.721    99.270   103.649          V2=   1123.74      -15.964    -25.797    -12.898
```

```
Sublattices for Delta = 1/ 2

                                  ***** Subcell   1 *****
```

```
T 1=       1.00    .00    .00/    .00   1.00    .00/    .00    .00    .50
T 2=        .00    .00    .50/   1.00    .00    .00/    .00   1.00    .00
T 2 INV=    .00   1.00    .00/    .00    .00   1.00/   2.00    .00    .00                    ** Cell Matrix **

CELL  1=   7.3932   7.3932   7.3932   76.351   76.351   76.351        V1=   374.58    13.665    54.659    54.659
CELL  2=   3.6966   7.3932   7.3932   76.351   76.351   76.351        V2=   187.29    12.898     6.449     6.449
```

```
                                  ***** Subcell   2 *****

T 1=       1.00    .00    .00/    .00   1.00    .00/    .00   -.50    .50
T 2=        .00   -.50    .50/    .00   -.50   -.50/   1.00    .00    .00
T 2 INV=    .00    .00   1.00/  -1.00  -1.00    .00/   1.00  -1.00    .00                    ** Cell Matrix **

CELL  1=   7.3932   7.3932   7.3932   76.351   76.351   76.351        V1=   374.58    20.880    33.779    54.659
CELL  2=   4.5695   5.8119   7.3932  107.468   90.000   90.000        V2=   187.29   -12.898      .000      .000
```

```
                                  ***** Subcell   3 *****

T 1=       1.00    .00    .00/    .00   1.00    .00/   -.50    .00    .50
T 2=        .50    .00   -.50/   -.50    .00   -.50/    .00   1.00    .00
T 2 INV=   1.00  -1.00    .00/    .00    .00   1.00/  -1.00  -1.00    .00                    ** Cell Matrix **

CELL  1=   7.3932   7.3932   7.3932   76.351   76.351   76.351        V1=   374.58    20.880    33.779    54.659
CELL  2=   4.5695   5.8119   7.3932  107.468   90.000   90.000        V2=   187.29   -12.898      .000      .000
```

```
                                  ***** Subcell   4 *****

T 1=       1.00    .00    .00/    .00   1.00    .00/   -.50   -.50    .50
T 2=       -.50   -.50    .50/   -.50    .50   -.50/    .50   -.50   -.50
T 2 INV=  -1.00  -1.00    .00/  -1.00    .00  -1.00/    .00  -1.00  -1.00                    ** Cell Matrix **

CELL  1=   7.3932   7.3932   7.3932   76.351   76.351   76.351        V1=   374.58    34.545    34.545    34.545
CELL  2=   5.8775   5.8775   5.8775  102.056  102.056  102.056        V2=   187.29    -7.216    -7.216    -7.216
```

```
                                  ***** Subcell   5 *****

T 1=       1.00    .00    .00/    .00    .50    .00/    .00    .00   1.00
T 2=        .00   -.50    .00/  -1.00    .00    .00/    .00    .00  -1.00
T 2 INV=    .00  -1.00    .00/  -2.00    .00    .00/    .00    .00  -1.00                    ** Cell Matrix **

CELL  1=   7.3932   7.3932   7.3932   76.351   76.351   76.351        V1=   374.58    13.665    54.659    54.659
CELL  2=   3.6966   7.3932   7.3932   76.351   76.351   76.351        V2=   187.29    12.898     6.449     6.449
```

```
                                  ***** Subcell   6 *****

T 1=       1.00    .00    .00/   -.50    .50    .00/    .00    .00   1.00
T 2=       -.50    .50    .00/    .50    .50    .00/    .00    .00  -1.00
T 2 INV=  -1.00   1.00    .00/   1.00   1.00    .00/    .00    .00  -1.00                    ** Cell Matrix **

CELL  1=   7.3932   7.3932   7.3932   76.351   76.351   76.351        V1=   374.58    20.880    33.779    54.659
CELL  2=   4.5695   5.8119   7.3932  107.468   90.000   90.000        V2=   187.29   -12.898      .000      .000
```

***** Subcell 7 *****

```
T 1=       .50    .00    .00/    .00   1.00    .00/    .00    .00   1.00
T 2=       .50    .00    .00/    .00   1.00    .00/    .00    .00   1.00
T 2 INV=  2.00    .00    .00/    .00   1.00    .00/    .00    .00   1.00                    ** Cell Matrix **

CELL  1=  7.3932  7.3932  7.3932  76.351  76.351  76.351        V1=  374.58   13.665  54.659  54.659
CELL  2=  3.6966  7.3932  7.3932  76.351  76.351  76.351        V2=  187.29   12.898   6.449   6.449
```

Sublattices for Delta = 1/ 3

***** Subcell 1 *****

```
T 1=      1.00    .00    .00/    .00   1.00    .00/    .00    .00    .33
T 2=       .00    .00    .33/  -1.00    .00    .33/    .00  -1.00    .33
T 2 INV=  1.00  -1.00    .00/   1.00    .00  -1.00/   3.00    .00    .00                    ** Cell Matrix **

CELL  1=  7.3932  7.3932  7.3932  76.351  76.351  76.351        V1=  374.58    6.073  52.133  52.133
CELL  2=  2.4644  7.2203  7.2203  78.524  84.279  84.279        V2=  124.86   10.373   1.774   1.774
```

***** Subcell 2 *****

```
T 1=      1.00    .00    .00/    .00   1.00    .00/    .00   -.33    .33
T 2=       .00   -.33    .33/    .00   -.33   -.67/   1.00    .00    .00
T 2 INV=   .00    .00   1.00/  -2.00  -1.00    .00/   1.00  -1.00    .00                    ** Cell Matrix **

CELL  1=  7.3932  7.3932  7.3932  76.351  76.351  76.351        V1=  374.58    9.280  36.099  54.659
CELL  2=  3.0463  6.0082  7.3932 106.880  90.000 104.686        V2=  124.86  -12.898    .000  -4.640
```

***** Subcell 3 *****

```
T 1=      1.00    .00    .00/    .00   1.00    .00/    .00   -.67    .33
T 2=       .00   -.33   -.33/    .00    .33   -.67/   1.00   -.33   -.33
T 2 INV= -1.00    .00   1.00/  -2.00   1.00    .00/  -1.00  -1.00    .00                    ** Cell Matrix **

CELL  1=  7.3932  7.3932  7.3932  76.351  76.351  76.351        V1=  374.58   15.013  24.634  52.474
CELL  2=  3.8746  4.9632  7.2439  84.883  76.790  67.025        V2=  124.86    3.207   6.414   7.506
```

***** Subcell 4 *****

```
T 1=      1.00    .00    .00/    .00   1.00    .00/   -.33    .00    .33
T 2=       .33    .00   -.33/   -.67    .00   -.33/    .00   1.00    .00
T 2 INV=  1.00  -1.00    .00/    .00    .00   1.00/  -2.00  -1.00    .00                    ** Cell Matrix **

CELL  1=  7.3932  7.3932  7.3932  76.351  76.351  76.351        V1=  374.58    9.280  36.099  54.659
CELL  2=  3.0463  6.0082  7.3932 106.880  90.000 104.686        V2=  124.86  -12.898    .000  -4.640
```

***** Subcell 5 *****

```
T 1=      1.00    .00    .00/    .00   1.00    .00/   -.33   -.33    .33
```

```
T 2=       -.33   -.33    .33/    .67   -.33    .33/   -.33    .67    .33
T 2 INV=  -1.00   1.00    .00/  -1.00    .00   1.00/   1.00   1.00   1.00                    ** Cell Matrix **

CELL  1=   7.3932   7.3932   7.3932    76.351   76.351   76.351        V1=   374.58    15.353   33.573   33.573
CELL  2=   3.9183   5.7942   5.7942   104.115   97.253   97.253        V2=   124.86    -8.188   -2.866   -2.866
```

***** Subcell 6 *****

```
T 1=       1.00    .00    .00/    .00   1.00    .00/   -.33   -.67    .33
T 2=        .33   -.33   -.33/    .33    .67   -.33/    .33   -.33    .67
T 2 INV=  1.00   1.00   1.00/  -1.00   1.00    .00/  -1.00    .00   1.00                    ** Cell Matrix **

CELL  1=   7.3932   7.3932   7.3932    76.351   76.351   76.351        V1=   374.58    15.353   33.573   33.573
CELL  2=   3.9183   5.7942   5.7942   104.115   97.253   97.253        V2=   124.86    -8.188   -2.866   -2.866
```

***** Subcell 7 *****

```
T 1=       1.00    .00    .00/    .00   1.00    .00/   -.67    .00    .33
T 2=       -.33    .00   -.33/   -.67    .00    .33/   -.33   1.00   -.33
T 2 INV=  -1.00  -1.00    .00/  -1.00    .00   1.00/  -2.00   1.00    .00                    ** Cell Matrix **

CELL  1=   7.3932   7.3932   7.3932    76.351   76.351   76.351        V1=   374.58    15.013   24.634   52.474
CELL  2=   3.8746   4.9632   7.2439    84.883   76.790   67.025        V2=   124.86     3.207    6.414    7.506
```

***** Subcell 8 *****

```
T 1=       1.00    .00    .00/    .00   1.00    .00/   -.67   -.33    .33
T 2=        .33   -.33    .33/   -.67   -.33    .33/    .33   -.33   -.67
T 2 INV=  1.00  -1.00    .00/  -1.00  -1.00  -1.00/   1.00    .00  -1.00                    ** Cell Matrix **

CELL  1=   7.3932   7.3932   7.3932    76.351   76.351   76.351        V1=   374.58    15.353   33.573   33.573
CELL  2=   3.9183   5.7942   5.7942   104.115   97.253   97.253        V2=   124.86    -8.188   -2.866   -2.866
```

***** Subcell 9 *****

```
T 1=       1.00    .00    .00/    .00   1.00    .00/   -.67   -.67    .33
T 2=       -.33   -.33   -.33/   -.67    .33    .33/    .33    .33   -.67
T 2 INV=  -1.00  -1.00    .00/  -1.00   1.00   1.00/  -1.00    .00  -1.00                    ** Cell Matrix **

CELL  1=   7.3932   7.3932   7.3932    76.351   76.351   76.351        V1=   374.58    26.819   27.840   27.840
CELL  2=   5.1787   5.2764   5.2764   120.000   90.000   90.000        V2=   124.86   -13.920     .000     .000
```

***** Subcell 10 *****

```
T 1=       1.00    .00    .00/    .00    .33    .00/    .00    .00   1.00
T 2=        .00   -.33    .00/   1.00   -.33    .00/    .00   -.33   1.00
T 2 INV=  -1.00   1.00    .00/  -3.00    .00    .00/  -1.00    .00   1.00                    ** Cell Matrix **

CELL  1=   7.3932   7.3932   7.3932    76.351   76.351   76.351        V1=   374.58     6.073   52.133   52.133
CELL  2=   2.4644   7.2203   7.2203    78.524   84.279   84.279        V2=   124.86    10.373    1.774    1.774
```

***** Subcell 11 *****

```
T 1=       1.00    .00    .00/   -.33    .33    .00/    .00    .00   1.00
T 2=       -.33    .33    .00/    .67    .33    .00/    .00    .00  -1.00
T 2 INV=  -1.00   1.00    .00/   2.00   1.00    .00/    .00    .00  -1.00                    ** Cell Matrix **

CELL  1=   7.3932    7.3932    7.3932     76.351    76.351    76.351        V1=   374.58      9.280    36.099    54.659
CELL  2=   3.0463    6.0082    7.3932     106.880    90.000    104.686       V2=   124.86    -12.898      .000    -4.640
```

***** Subcell 12 *****

```
T 1=       1.00    .00    .00/   -.67    .33    .00/    .00    .00   1.00
T 2=        .33    .33    .00/    .67   -.33    .00/    .33    .33  -1.00
T 2 INV=   1.00   1.00    .00/   2.00  -1.00    .00/   1.00    .00  -1.00                    ** Cell Matrix **

CELL  1=   7.3932    7.3932    7.3932     76.351    76.351    76.351        V1=   374.58     15.013    24.634    52.474
CELL  2=   3.8746    4.9632    7.2439     84.883    76.790    67.025        V2=   124.86      3.207     6.414     7.506
```

***** Subcell 13 *****

```
T 1=        .33    .00    .00/    .00   1.00    .00/    .00    .00   1.00
T 2=        .33    .00    .00/    .33  -1.00    .00/    .33    .00  -1.00
T 2 INV=   3.00    .00    .00/   1.00  -1.00    .00/   1.00    .00  -1.00                    ** Cell Matrix **

CELL  1=   7.3932    7.3932    7.3932     76.351    76.351    76.351        V1=   374.58      6.073    52.133    52.133
CELL  2=   2.4644    7.2203    7.2203     78.524    84.279    84.279        V2=   124.86     10.373     1.774     1.774
```

IV. Cell transformation

A. Introduction

This program function enables the user to transform a unit cell by a specified three by three matrix.

B. Operation of the program

1. General

There are three types of input lines required to execute the cell transformation (TRANS) program function. The first input line is a Program Control Line that specifies the type of program function and the number of independent problems to be considered. The second type of input line is a Matrix Parameter Line that defines the matrix to be used to transform the unit cell. The final type of input line is the Cell Parameter Line that specifies the unit cell parameters a,b,c, alpha, beta, gamma. For N problems specified on the Program Control Line, N sets of lines consisting of one Matrix Parameter Line followed by one Cell Parameter Line must be input to the program. Within a single computer run, the TRANS program function may be executed any number of times. A description of the formats for the input lines and typical examples are given below.

2. Description of input lines

a. Program Control Line

The Program Control Line specifies the type of program function and the number of problems to be solved. For each execution of the TRANS program function within a single computer run, only one Program Control Line is required.

Program Control Line
Format(A5,3X,I2)

	Column	Format	Item
1	1–5	A5	Type of program function 'LM ' = Lattice Matching 'RSS ' = Reduction and Derivative Supercell and Subcell 'TRANS' = Cell Transformation 'INV ' = Matrix Inversion
	6–8	3X	Blank
2	9–10	I2	Number of problems

Notes:

1 The TRANS program function is specified by 'TRANS' in columns 1–5.

2 The number of problems specified in a single execution of the TRANS program function may range between 1 and 99.

b. Matrix Parameter Line

The Matrix Parameter Line defines the matrix to be used to transform the unit cell. The form of the three by three transformation matrix required to execute the TRANS program function is :

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} .$$

The Matrix Parameter Line must precede the Cell Parameter Line.

Matrix Parameter Line
Format(9F8.2)

	Column	Format	Item
1	1–8	F8.2	Matrix element a_{11}
2	9–16	F8.2	Matrix element a_{12}
3	17–24	F8.2	Matrix element a_{13}
4	25–32	F8.2	Matrix element a_{21}
5	33–40	F8.2	Matrix element a_{22}
6	41–48	F8.2	Matrix element a_{23}
7	49–56	F8.2	Matrix element a_{31}
8	57–64	F8.2	Matrix element a_{32}
9	65–72	F8.2	Matrix element a_{33}

Notes:

1–9 Each matrix element must be represented as a decimal number.

c. Cell Parameter Line

This input line is used to define the unit cell to be transformed. All six unit cell parameters must always be specified regardless of the crystal symmetry. The Cell Parameter Line must follow the Matrix Parameter Line.

Cell Parameter Line
Format(10X,6F10.5)

	Column	Format	Item
	1–10	10X	Blank
1	11-20	F10.5	a (Å)
2	21–30	F10.5	b
3	31–40	F10.5	c
4	41–50	F10.5	alpha (°)
5	51–60	F10.5	beta
6	61–70	F10.5	gamma

Notes:

1–3 Cell edges (Å).

4–6 Cell angles (degrees). Decimal numbers must be used for fractions of a degree.

3. Example of input flowstream

```
.........1.........1.........1.........1.........1.........1.........1

1   TRANS    2
2   .0      1.0      .0       .0       1.0      -2.0     -1.0     .0       .0
3              5.674      6.282      8.225      67.55      81.05      65.96
4   1.0     2.0      1.0      .0       -1.0     1.0      1.0      .0       .0
5              10.864     16.110     16.110     115.10     102.99     102.99
```

Notes:

1 The 'TRANS' in columns 1–5 indicates that the TRANS program function will be executed. The '2' in column 10 specifies that two independent problems are to be considered. This means that two sets of lines consisting of one Matrix Parameter Line followed by one Cell Parameter Line must be input to the program.

2 This input line defines the matrix to be used to transform the first input cell.

3 All six unit cell parameters must be specified regardless of the crystal symmetry. Cell edges are in angstroms and cell angles are in degrees. Decimal numbers have been used for fractions of a degree. This unit cell will be transformed by the matrix defined on the second input line.

4 This input line defines the matrix to be used to transform the second input cell.

5 All six unit cell parameters are specified on this input line. Cell edges are in angstroms and cell angles are in degrees. Decimal numbers have been used for fractions of a degree. This unit cell will be transformed by the matrix defined on the fourth input line.

4. Example of computer output

The computer output following this section results from the input flowstream discussed above (sec. IV.B.3). A description of the output parameters is printed for the first execution of the TRANS program function within a computer run.

For the first independent problem (Cell Transformation 1), the input cell (CELL 1) was the reduced cell. The input matrix (T2), taken from table 3 in section III, transforms the reduced cell (reduced form number 30) to a C-centered monoclinic cell (CELL 2). The input cell for the second independent problem (Cell Transformation 2) was also the reduced cell (reduced form number 24). The input matrix, T2, transforms the reduced cell to the triply primitive rhombohedral cell (metrically hexagonal axes).

Example
Section IV.

```
                    *** NBS*LATTICE ***

          A PROGRAM TO ANALYZE LATTICE RELATIONSHIPS
                  Version of Spring, 1985

                    NBS Crystal Data Center
                  National Bureau of Standards
                  Reactor Radiation Division
                    Gaithersburg, MD  20899
```

```
                ** CELL TRANSFORMATION **

      CELL 1   =   Input cell.
      CELL 2   =   Transformed cell.
      T 2      =   Input transformation matrix.
      T 2 INV  =   Inverse matrix for T 2.

   For CELL 1 and CELL 2, the output parameters given are:
       a, b, c, alpha, beta, gamma and volume.  Cell edges
       are in angstroms and angles in degrees.

   The cell matrix is of the form:      a.a   b.b   c.c
                                        b.c   a.c   a.b
```

CELL TRANSFORMATION

** Cell Transformation 1 **

```
T 2=        .00   1.00    .00/    .00   1.00  -2.00/  -1.00    .00    .00
T 2 INV=    .00    .00  -1.00/   1.00    .00    .00/    .50   -.50    .00
```

** Cell Matrix **

```
CELL  1=   5.6740    6.2820    8.2250     67.550     81.050     65.960        V1=   247.45     39.464   231.141    32.194
CELL  2=   6.2820   15.2033    5.6740     90.000    114.040     90.000        V2=   494.90      .000    -14.520      .001
```

** Cell Transformation 2 **

```
T 2=        1.00   2.00   1.00/    .00  -1.00   1.00/   1.00    .00    .00
T 2 INV=     .00    .00   1.00/    .33   -.33   -.33/    .33    .67   -.33
```

** Cell Matrix **

```
CELL  1=  10.8640   16.1100   16.1100    115.100    102.990    102.990        V1=  2318.45    739.268   739.251   118.026
CELL  2=  27.1895   27.1892   10.8640     90.000     89.999    120.000        V2=  6955.35      .000      .004  -369.625
```

V. Matrix inversion

A. Introduction

This program function enables the user to calculate the inverse of a three by three matrix.

B. Operation of the program

1. General

There are two types of input lines required to execute the matrix inversion (INV) program function. The first input line is a Program Control Line that specifies the type of program function and the number of independent problems to be considered. The second type of input line is a Matrix Parameter Line that defines the matrix whose inverse (if one exists) is to be calculated. For N problems specified on the Program Control Line, N Matrix Parameter Lines must follow. Within a single computer run, the INV program function may be executed any number of times. A description of the formats for the input lines and typical examples follow.

2. Description of input lines

a. Program Control Line

The Program Control Line specifies the type of program function and the number of problems to be considered. For each execution of the INV program function within a single computer run, only one Program Control Line is required.

Program Control Line
Format(A5,3X,I2)

	Column	Format	Item
1	1–5	A5	Type of program function 'LM ' = Lattice Matching 'RSS ' = Reduction and Derivative Supercell and Subcell 'TRANS' = Cell Transformation 'INV ' = Matrix Inversion
	6–8	3X	Blank
2	9–10	I2	Number of problems

Notes:

1 The INV program function is specified by 'INV ' in columns 1–5.

2 The number of problems specified in a single execution of the INV program function may range between 1 and 99.

b. Matrix Parameter Line

The Matrix Parameter Line defines the matrix whose inverse is to be calculated. The form of the three by three matrix is:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} .$$

For N problems specified on the Program Control Line, N Matrix Parameter Lines must be input to the program.

Matrix Parameter Line
Format(9F8.2)

	Column	Format	Item
1	1–8	F8.2	Matrix element a_{11}
2	9–16	F8.2	Matrix element a_{12}
3	17–24	F8.2	Matrix element a_{13}
4	25–32	F8.2	Matrix element a_{21}
5	33–40	F8.2	Matrix element a_{22}
6	41–48	F8.2	Matrix element a_{23}
7	49–56	F8.2	Matrix element a_{31}
8	57–64	F8.2	Matrix element a_{32}
9	65–72	F8.2	Matrix element a_{33}

Notes:

1–9 Each matrix element must be represented as a decimal number.

3. Example of input flowstream

```
.........1.........1.........1.........1.........1.........1.........1
```

```
1   INV       2
2   -1.0      .0        .0        .0        -1.0      1.0       -1.0      1.0       1.0
3   1.0       -1.0      .0        -1.0      .0        1.0       -1.0      -1.0      -1.0
```

Notes:

1 The 'INV ' in columns 1–5 indicates that the INV program function will be executed. The '2' in column 10 specifies that two independent problems are to be considered. Thus, two Matrix Parameter Lines follow the Program Control Line.

2–3 Each matrix element has been specified by a decimal number.

4. Example of computer output

The computer output following this section results from the input flowstream discussed above (sec. V.B.3.). A description of the output parameters is printed for the first execution of the INV program function within a computer run. The two matrices used in this example were taken from table 3 in section III. The input matrix (T2) for the first independent problem (Matrix Inversion 1) transforms a reduced cell having reduced form number 19 to an I-centered orthorhombic cell. The input matrix for the second independent problem (Matrix Inversion 2) transforms a reduced cell having reduced form number 2 to a triply primitive rhombohedral cell (metrically hexagonal axes).

Example
Section V.

```
                              ***  NBS*LATTICE  ***

                        A PROGRAM TO ANALYZE LATTICE RELATIONSHIPS
                                 Version of Spring, 1985

                                  NBS Crystal Oata Center
                                National Bureau of Standards
                                Reactor Radiation Oivision
                                  Gaithersburg, MO  20899
```

```
                    ** MATRIX INVERSION **

          T 2      =   Input transformation matrix.
          T 2 INV  =   Inverse matrix for T 2.
```

```
          MATRIX INVERSION
```

```
                                ** Matrix Inversion  1 **

T 2=      -1.00    .00    .00/    .00  -1.00   1.00/  -1.00   1.00   1.00
T 2 INV=  -1.00    .00    .00/   -.50   -.50    .50/   -.50    .50    .50
```

```
                                ** Matrix Inversion  2 **

T 2=       1.00  -1.00    .00/  -1.00    .00   1.00/  -1.00  -1.00  -1.00
T 2 INV=    .33   -.33   -.33/   -.67   -.33   -.33/    .33    .67   -.33
```

VI. Summary of program operations

A. General

The *NBS*LATTICE* program is designed for use in any analytical laboratory. The program uses metric methods to analyze various types of lattice relationships. Whenever using metric methods, one must be particularly careful that the unit cell parameters and errors have been properly determined and interpreted. In many cases, it appears that the reported experimental error is too optimistic, even for unit cell parameters refined by least-squares analysis using modern diffractometry. Independent unit cell determinations of beta-clopenthixol illustrate this point. The x-ray crystal structure of beta-clopenthixol has been reported in the literature (Jones, Sheldrick & Horn, 1981). Previously, a crystalline sample of beta-clopenthixol had been obtained from one of the authors (A.H.) and the unit cell parameters were determined using both powder (Morris, McMurdie, Evans, Paretzkin, Hubbard & Carmel, 1980) and single-crystal (Himes, 1983) diffraction techniques.

Published single-crystal cell	Single-crystal cell	Powder cell
a = 6.493(2) Å	6.4978(7) Å	6.518(4) Å
b = 7.758(3)	7.7701(8)	7.773(3)
c = 21.881(8)	21.871(2)	21.939(11)
α = 90.11(2) °	90.011(8) °	90.06(4) °
β = 91.48(2)	91.501(9)	91.60(5)
γ = 92.81(2)	93.129(9)	93.06(4)

A comparison of the unit cell parameters reveals that they are in reasonable agreement with each other. However, depending on which values are used, the gamma angles for the two cells refined on diffractometers differ by approximately 16 to 35 estimated standard deviations. Thus, in general, one should assume rather large experimental errors when analyzing lattice relationships. This is especially true when working with cells prior to the final cell, or for cases in which unit cell parameters were determined from irregularly shaped crystals having an absorption problem.

The present version of *NBS*LATTICE* performs several functions including: 1) the characterization and identification of unknown materials using lattice-formula matching techniques; 2) the calculation of the reduced cell of the lattice, and the calculation and reduction of specified derivative supercells and/or subcells; 3) unit cell transformations; and 4) matrix inversions. To execute the lattice-matching (LM) program function, three types of input lines are required. For N problems specified on the Program Control Line, one LM Parameter Line and N RSS Control Lines must follow ($1 \leq N \leq 20$). Within a single computer run, the LM program function may be executed only once. Although at most 20 independent problems may be considered, up to 900 lattices may be matched against data from the *NBS Crystal Data File* in a single run. To execute the reduction and derivative supercell and subcell (RSS) program function, two types of input lines are required. For N problems specified on the Program Control Line, N RSS Control Lines must follow ($1 \leq N \leq 20$). There are three types of input lines required to execute the cell transformation (TRANS) program function. For N problems specified on the Program Control Line, N sets of lines consisting of one Matrix Parameter Line followed by one Cell Parameter Line must be input to the program ($1 \leq N \leq 99$). The execution of the matrix inversion (INV) program function requires two types of input lines. For N problems specified on the Program Control Line, N Matrix Parameter Lines must follow ($1 \leq N \leq 99$). The RSS, TRANS, and INV program functions may be executed any number of times within a single computer run. A description of the formats for the input lines is given below.

B. Description of input lines

Each individual section II through V contains additional information concerning the theory and operations for each program function.

1. Program Control Line

The Program Control Line specifies the type of program function and the number of independent problems to be considered. One Program Control Line is required for each program function to be executed.

Program Control Line
Format(A5,3X,I2)

Column	Format	Item
1–5	A5	Type of program function 'LM ' = Lattice Matching 'RSS ' = Reduction and Derivative Supercell and Subcell 'TRANS' = Cell Transformation 'INV ' = Matrix Inversion
6–8	3X	Blank
9–10	I2	Number of problems

2. LM Parameter Line

The LM Parameter Line specifies the tolerances for a match of a,b,c, and V, the file(s) to be searched, and whether full or limited output is desired. Tolerances of 0.10 Å and 10.0 percent are reasonable values to specify for most problems. The user may wish to increase these tolerances in a second run depending on the results obtained. Only one LM Parameter Line is allowed when executing the LM program function.

LM Parameter Line
Format(2F10.2,5X,5A1,9X,I1)

Column	Format	Item	
1–10	F10.2	Tolerance for a match of the cell edges (Å)	
11–20	F10.2	Tolerance for a match of the cell volume (percentage of $Å^3$)	
21–25	5X	Blank	
26–30	5A1	I/O/	Inorganic/Organic/ May specify one or more files to be searched.
31–39	9X	Blank	
40	I1	Blank/1/	Print/Do not print/ RSS output

3. RSS Control Line

The RSS Control Line defines the input lattice and the derivative lattices to be calculated. To define the lattice, the cell centering and all six unit cell parameters (regardless of the crystal symmetry) must be specified. When executing the LM program function, especially when some chemical information is known, it is recommended to check routinely for the 55 supercells of 2, 3, and 4 times the volume and the 55 subcells of 1/2, 1/3, and 1/4 times the volume of the reduced input cell.

RSS Control Line
Format(I1,2X,2I1,3X,2A1,6F10.2)

Column	Format	Item
1	I1	Blank/1/2/3/ Blank = Reduction 1 = Reduction + supercells 2 = Reduction + subcells 3 = Reduction + supercells, subcells
2–3	2X	Blank
4	I1	Blank/2/3/4/5/6/7/8/9/ Initial value (n1) to define the range of volumes for calculated derivative lattices.
5	I1	Blank/2/3/4/5/6/7/8/9/ Final value (n2) to define the range of volumes for calculated derivative lattices.
6–8	3X	Blank
9	A1	P/A/B/C/F/I/R/ Cell centering
10	A1	R/H/ Rhombohedral/Hexagonal/ metric axes. Used only for rhombohedral lattices.
11–20	F10.2	a (Å)
21–30	F10.2	b
31–40	F10.2	c
41–50	F10.2	alpha (°)
51–60	F10.2	beta
61–70	F10.2	gamma

4. Matrix Parameter Line

The Matrix Parameter Line defines the three by three matrix to be used when executing the TRANS or INV program functions.

Matrix Parameter Line
Format(9F8.2)

Column	Format	Item
1–8	F8.2	Matrix element a_{11}
9–16	F8.2	Matrix element a_{12}
17–24	F8.2	Matrix element a_{13}
25–32	F8.2	Matrix element a_{21}
33–40	F8.2	Matrix element a_{22}
41–48	F8.2	Matrix element a_{23}
49–56	F8.2	Matrix element a_{31}
57–64	F8.2	Matrix element a_{32}
65–72	F8.2	Matrix element a_{33}

5. Cell Parameter Line

This input line is used to define a unit cell. All six unit cell parameters must always be specified regardless of the crystal symmetry.

Cell Parameter Line
Format(10X,6F10.5)

Column	Format	Item
1–10	10X	Blank
11–20	F10.5	a (Å)
21–30	F10.5	b
31–40	F10.5	c
41–50	F10.5	alpha (°)
51–60	F10.5	beta
61–70	F10.5	gamma

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Appendix I. *NBS Crystal Data File*

A large data base with chemical and crystallographic data is available for lease in magnetic tape form. The data base contains evaluated data on approximately 60,000 materials. The data are collected from the published literature. To avoid duplication of effort, the NBS Crystal Data Center collaborates with other data centers including the Cambridge Crystallographic Data Centre (England); the JCPDS-International Centre for Diffraction Data (Swarthmore, PA); the Metals Data Center (Ottawa, Canada); and the Inorganic Structural Data Center (Bonn, Germany). The NBS Crystal Data Center is especially interested in the nature of the lattice and the chemical composition. The data for each compound are processed, evaluated, and put into standard form. Derivative parameters are calculated such as the reduced cell, the empirical formula and the calculated density. Each entry consists of the reduced cell and volume, crystal system, space group, space group number, density, chemical name, chemical formula, reference to *Crystal Data*, journal reference, plus additional data. The work was supported by the Office of Standard Reference Data at the National Bureau of Standards.

Use of the Data Base

The data base will prove to be a practical analytical tool for compound identification because the reduced cell in the lower symmetry crystal systems or the reduced cell plus some chemical data in the higher symmetry crystal systems is unique for most compounds. Unknowns can conveniently be identified by the following sequence:

1. Determine a primitive or centered cell for the unknown crystal;
2. Calculate the reduced cell;
3. Check the *NBS Crystal Data File*;
4. Identify the unknown compound on the basis of the lattice (as defined by the unit cell parameters) and/or chemical information.

In addition to routine analytical work, the data base will be useful in research studies and in preventing redeterminations of published structures.

Coverages and Updates

The data base contains data for most commonly occurring materials. All types of substances with known unit cells are included. The data fall into the following categories: organics, organometallics, metals, intermetallics, inorganics, and minerals. New entries are being added on a regular basis and a revised version of the data base will be made available to users on a periodic basis.

Information

For questions concerning the scientific content of the File, write the NBS Crystal Data Center. Distribution of the *NBS Crystal Data File* is being handled by:

JCPDS-International Centre for Diffraction Data
1601 Park Lane
Swarthmore, PA 19081
Telephone: 215-328-9400 .

Structure of an Entry

Each entry consists of the data for one crystalline compound. Each entry consists of the reduced cell, cell volume, crystal system, space group, space group number, calculated density, chemical name, chemical formula, and journal reference. There are four record types (i.e., four 80 character records) per entry:

Record 1 Reduced Cell and References
Record 2 Space Group, Calculated Density, Chemical Class, Reduced Cell Volume
Record 3 Chemical Formula
Record 4 Chemical Name.

Record 3 and record 4 can be continued. All records in a given entry have the same identification number.

Format Specifications for Each Record in an Entry

RECORD 1 REDUCED CELL and REFERENCES

Column	Format	Item
1–6	F6.2	a (reduced cell)
7–12	F6.2	b
13–18	F6.2	c
19–24	F6.1	alpha
25–30	F6.1	beta
31–36	F6.1	gamma
37	1X	Blank
38	I1	*Crystal Data* volume number
39	A1	Crystal system (A, M, O, R, T, H, C)
40–48	F9.4	*Crystal Data* ratio
49	1X	Blank
50–55	A6	CODEN for journal reference
56–59	A4	Volume
60	1X	Blank
61–64	A4	Page
65	1X	Blank
66–69	I4	Year
70	1X	Blank
71	A1	Structure code (N, L, T)
72	A1	* (If quant. structure occurs in a different reference; inorganic file only)
73–78	6A1	ID number
79	1X	Blank
80	A1	1

RECORD 2 SPACE GROUP, D*x*, CLASS, REDUCED CELL VOLUME

Column	Format	Item
1–3	I3	Space group number
4	1X	Blank
5–12	A8	*Crystal Data* space group
13	1X	Blank
14–18	F5.2	D*x*
19	1X	Blank
20–22	A3	Chemical class
23	1X	Blank
24–32	I9	Reduced cell volume
33–34	2X	Blank
35–42	A8	Accession date
43–44	2X	Blank
45–52	A8	Modification date
53–72	20X	Blank
73–78	6A1	ID number
79	1X	Blank
80	I1	2

RECORD 3 CHEMICAL FORMULA

Column	Format	Item
1–67	67A1	Chemical formula
68–69	2X	Blank
70	A1	C (formula continuation code)
71	I1	Sequence number
72	1X	Blank
73–78	6A1	ID number
79	1X	Blank
80	I1	3

RECORD 4 CHEMICAL NAME

Column	Format	Item
1–67	67A1	Chemical name
68–69	2X	Blank
70	A1	C (name continuation code)
71	I1	Sequence number
72	1X	Blank
73–78	6A1	ID number
79	1X	Blank
80	I1	4

Description of Data Parameters for Record 1

1. Reduced Cell Cols. 1–36

   The reduced cell is a unique, primitive cell that is based on the three shortest vectors of the lattice. The cell edges are set so that $a \leq b \leq c$. The mathematical conditions for full reduction and procedures to obtain the reduced cell have been published (Santoro & Mighell, 1970; *International Tables for X-ray Crystallography*, 1969 *a*).

2. *Crystal Data* Volume Number Col. 38

   This is the volume number (1–6) in the *Crystal Data: Determinative Tables* (1972, 1973, 1978, 1984) series in which additional data on the compound may be found. This number is given only for inorganic entries.

3. Crystal System Col. 39

   A = Anorthic (Triclinic)
   M = Monoclinic
   O = Orthorhombic
   R = Rhombohedral
   T = Tetragonal
   H = Hexagonal
   C = Cubic.

4. *Crystal Data* Ratio Cols. 40–48

The first determinative ratio for the cell reported on the top line in *Crystal Data: Determinative Tables* is given. The first determinative ratio is:

a/b = Anorthic, monoclinic, and orthorhombic
c/a = Tetragonal and hexagonal
c/a = Rhombohedral (metrically hexagonal axes)
a = Cubic.

5. Journal Reference Cols. 50–69

The journal reference to the original literature from which the data were extracted is given as: CODEN (i.e. a code representing the journal name), volume, page, year. Most CODENS correspond to those used by Chemical Abstracts, a few have been made up by the data center. A file of CODENS and journal names is distributed with the *NBS Crystal Data File*.

6. Structure Code (N, L, T) Col. 71

'T' signifies that a full structure determination has been reported in the original literature. Usually all parameters except hydrogen have been refined.

'N' signifies structural data have not been given.

'L' signifies that limited structural data have been reported.

7. Full Structure Determination Reported in a Different Reference Col. 72

If a '*' occurs in col. 72, it signifies that another reference reports a full structure determination on the same material. This symbol is used only for inorganic data.

8. ID Number Cols. 73–78

Each entry has a unique identification number. All records in a given entry have the same identification number.

9. Record Sequence Number Col. 80

A sequence number of 1,2,3,4 is used for record types 1–4.

Description of Data Parameters for Record 2

1. Space Group Number Cols. 1–3

A number (1–230) as given in Volume 1 of the *International Tables for X-ray Crystallography* (1969 *b*).

2. *Crystal Data* Space Group Cols. 5–12

The conventional space group symbol which corresponds to the cell setting as given on the top line of each entry in *Crystal Data: Determinative Tables*. A list of all possible symbols is given in NBS Technical Note 1141 (Mighell, Hubbard & Stalick, 1981).

3. D*x* (Calculated Density) Cols. 14–18

4. Chemical Class Cols. 20–22

   For the inorganic compounds, an 'M' is given if the compound is a mineral. For the organic compounds, the chemical class is specified by a number 1–86. Each number corresponds to a chemical class as listed in *Molecular Structures and Dimensions* (1970–1984).

   Examples: 18 = Benzoquinones; 51 = Steroids

5. Reduced Cell Volume Cols. 24–32

   Cell volume ($Å^3$) of the primitive reduced cell given on record 1.

6. Accession and Modification Dates Cols. 35–52

   These two dates are used by the Data Center for internal bookkeeping.

7. ID Number Cols. 73–78

   Same unique identification number as on record 1.

8. Record Sequence Number Col. 80

   Always a '2'.

Description of Data Parameters for Record 3

1. Chemical Formula Cols. 1–67

   The formula is expressed by a sequence of discrete units. For a complete description of the conventions used in the data base, see NBS Technical Note 1141.

2. Continuation Code and Sequence No. Cols. 71–72

   If more than one record is required for the formula, the symbols in columns 70 and 71 are nonblank.
   Example:

	Col. 70	Col. 71
Formula _____	C	1
Formula _____	C	2
Formula _____		3

3. ID Number Cols. 73–78

   Same unique identification number as on records 1 and 2.

4. Record Sequence Number Col. 80

   Always a '3'.

Description of Data Parameters for Record 4

1. Chemical Name Cols. 1–67

   For inorganic compounds, the numbers following the name indicate the number of atoms (or radicals) corresponding to each word in the name.
   Example:

   Iron Nitride (3 1) = Fe_3 N
   Zirconium Bromide Nitride (1 1 1) = Zr Br N

   For organic compounds, the names as given in the literature have not been modified.

2. Continuation Code and Sequence No. Cols. 71–72

   Same as for record 3 (item 4).

3. ID Number Cols. 73–78

   Same unique identification number as on records 1,2, and 3.

4. Record Sequence Number Col. 80

   Always a '4'.

Appendix II. 1-Line Search File

The 1-Line Search File contains crystallographic and chemical data on approximately 60,000 materials. This data file contains selected lattice and chemical data which were derived from the *NBS Crystal Data File* (see app. I).

Structure of an Entry

Each entry corresponds to the data for one crystalline compound. Each entry consists of the reduced cell, cell volume, space group number, crystal system, structure code, sequence number, journal reference, and chemical formula. There is one record (132 characters) per entry.

Format Specifications

Column	Format	Item
1–6	F6.2	a (reduced cell)
7–12	F6.2	b
13–18	F6.2	c
19–24	F6.1	alpha
25–30	F6.1	beta
31–36	F6.1	gamma
37–42	I6	Reduced cell volume
43	1X	Blank
44–46	I3	Space group number
47	1X	Blank
48	A1	Crystal system (A, M, O, R, T, H, C)
49	A1	Structure code (N, L, T)
50	1X	Blank
51–55	I5	Sequence number
56	1X	Blank
57–62	A6	CODEN for journal reference
63–66	A4	Volume
67	1X	Blank
68–71	A4	Page
72	1X	Blank
73–76	A4	Year
77	1X	Blank
78–131	A54	Chemical formula
132	A1	Truncation symbol for chemical formula

Description of Data Parameters

1. Reduced Cell Cols. 1–36

   The reduced cell is a unique, primitive cell that is based on the three shortest vectors of the lattice. The cell edges are set so that $a \leq b \leq c$. The mathematical conditions for full reduction and procedures to obtain the reduced cell have been published.

2. Reduced Cell Volume Cols. 37–42

   Cell volume ($Å^3$) of the primitive reduced cell.

3. Space Group Number Cols. 44–46

   A number (1–230) as given in Volume 1 of the *International Tables for X-ray Crystallography* (1969 *b*).

4. Crystal System Col. 48

A = Anorthic (Triclinic)
M = Monoclinic
O = Orthorhombic
R = Rhombohedral
T = Tetragonal
H = Hexagonal
C = Cubic.

5. Structure Code (N, L, T) Col. 49

'T' signifies that a full structure determination has been reported in the original literature. Usually all parameters except hydrogen have been refined.

'N' signifies structural data have not been given.

'L' signifies that limited structural data have been reported.

6. Sequence Number Cols. 51–55

The position of the entry in the 1-Line Search File.

7. Journal Reference Cols. 57–76

The journal reference to the original literature from which the data were extracted is given as: CODEN (i.e., a code representing the journal name), volume, page, year. Most CODENS correspond to those used by Chemical Abstracts, a few have been made up by the data center. A file of CODENS and journal names is distributed with the *NBS Crystal Data File*.

8. Chemical Formula Cols. 78–131

The formula is expressed by a sequence of discrete units. For a complete description of the conventions used in the data base, see NBS Technical Note 1141.

9. Truncation Symbol Col. 132

A '*' signifies that the chemical formula has been truncated to 54 characters.

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FORM NBS-114A (REV.11-84)

U.S. DEPT. OF COMM. **BIBLIOGRAPHIC DATA SHEET** (See instructions)	1. PUBLICATION OR REPORT NO. NBS/TN-1214	2. Performing Organ. Report No.	3. Publication Date December 1985

4. TITLE AND SUBTITLE

NBS*LATTICE A Program to Analyze Lattice Relationships

5. AUTHOR(S)

Vicky L. Himes and Alan D. Mighell

6. PERFORMING ORGANIZATION (If joint or other than NBS, see instructions)

NATIONAL BUREAU OF STANDARDS
U.S. DEPARTMENT OF COMMERCE
GAITHERSBURG, MD 20899

7. Contract/Grant No.

8. Type of Report & Period Covered

Final

9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS (Street, City, State, ZIP)

Same as item 6

10. SUPPLEMENTARY NOTES

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

A FORTRAN program to analyze lattice relationships has been written and is available for distribution by the NBS Crystal Data Center. The present version of *NBS*LATTICE* performs several functions including: 1) the characterization and identification of unknown materials using lattice-formula matching techniques; 2) the calculation of the reduced cell of the lattice, and the calculation and reduction of specified derivative supercells and/or subcells (i.e., this program function calculates the standard cells which are useful in the determination of metric lattice symmetry, in finding a matrix relating two unit cells, etc.); 3) unit cell transformations; and 4) matrix inversions. It is planned to incorporate additional functions in forthcoming versions of this program. Among others, these functions will include a matrix method to determine metric lattice symmetry and a technique to find a transformation matrix relating any two unit cells.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

computer program; lattice; identification; reduction; supercell; subcell; symmetry; transformation; data base

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